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A METHODOLOGY FOR QUANTITATIVE COMPARISON OF EXPERIMENTAL TO PREDICTED CHEMICAL DEPOSITION DATA

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Evaluation techniques were developed to assess computer simulation of single chemical munition field trials. These techniques were used to quantitatively compare the predicted to experimental deposition data. The methods employed for evaluating single munitions are not appropriate for the multiple munition field trials that are currently being conducted. Hence, the data fitting techniques were re-examined and new methodology developed that could be applied regardless of the number of munitions tested. The statistical tests chosen were the Sign, Mann-Whitney U, and Chi-Square tests. An additional metric was a modified version of the Chi-Square, referred to as the Point-by-Point. Each test was exercised using data from eleven field trials to test its appropriateness for this application. A best-fit criterion was established based on the evaluation of the test results.

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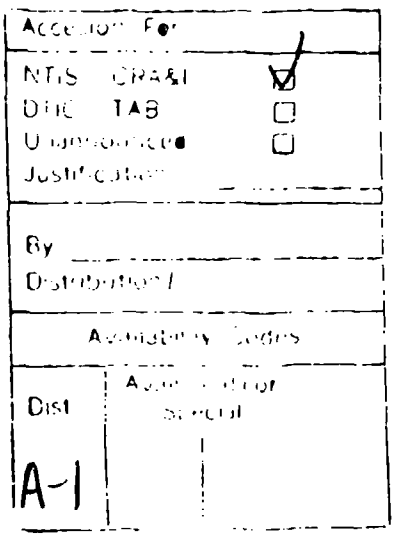

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I. INTRODUCTION

Evaluation techniques were developed to assess computer simulation of chemical simulant munition field trials. [1] These techniques were used to quantitatively compare the predicted to experimental deposition data for single munitions. The methods employed for evaluating single munitions are not appropriate for the multiple munition field trials currently being conducted. Hence, the data fitting techniques were re-examined and a new methodology developed that could be applied regardless of the number of munitions tested. A brief background discussion is provided to aid in understanding the intended purpose of this analysis.

II. BACKGROUND

1. Chemical Munition Analyses

a. **Single Munition.** In previous analyses, a single chemical munition was under investigation. A computer code called BIND was used to compare the computer generated ground deposition to the experimental deposition data. Data analysis techniques in BIND utilize metrics which considered both area and geometry of the two-dimensional pattern on the ground at user specified deposition levels. These deposition patterns are referred to as contours (iso-deposition curves). The geometry of the pattern was described in terms of the major axis which was defined as the length of the pattern measured in the downwind direction. BIND also provided graphical output of the predicted and experimental deposition contours. Visual inspection of these contours at the user specified deposition levels aided in assessing the goodness of the computer prediction.

b. **Multiple Munitions.** In analyzing multiple munition field trials, it was determined that the metrics used for the single munition analysis were not appropriate. For contours generated from multiple munitions, the major axis is not clearly defined because the shape is subject to the relative placement of one munition to another. Overlaying of contours from multiple munitions must be considered when describing the shape of the entire pattern; the major axis does not describe this phenomena. Therefore, other means of evaluating the computer prediction were investigated through the use of additional quantitative tests. These tests were implemented in an interactive graphic computer program called MULTI

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1. Klopcic, J. Terrence and Hindman, Tracy P., *Deposition Modeling and Effectiveness Evaluation Using Chemical Weapon Field Trial Dispersion Data*, U.S. Army Ballistic Research Laboratory, Technical Report BRL-MR-3652, March 1988, (Unclassified).

2. Experimental and Predicted Data

To evaluate the fitting procedures, experimental and computer generated data for eleven field trials were examined. Experimental data collected from field trials conducted at Dugway Proving Ground (DPG) included dissemination data, optical and radar tracking data of the munition from time of function to impact, and meteorological data. Dissemination data can be collected in various ways. For this analysis, data collection consisted of a 50 by 50 array of filter paper samplers placed 100 meters apart on a 3 mile by 3 mile grid, as shown in Figure A-1 of Appendix A. The meteorological data included temperature, Pasquill Stability category, and wind speed and direction as measured from two tower locations. A thirty minute summary of the meteorological data along with supplemental data was reported.

The Non Uniform Simple Surface Evaporation (NUSSE3) model was used to replicate the liquid (simulant) ground [illegible]tion patterns by describing the transport and diffusion of chemical agen[illegible] into the lower atmosphere.[2,3] A subset of DPG data, for example the [illegible]gical and trajectory data, was used to obtain the necessary inputs for N[illegible] the remaining inputs were derived mathematically from the initial conditions o. the test. The initial set of NUSSE3 inputs was referred to as the baseline. For example, the thirty minute summary of the meteorological data provided the baseline meteorological conditions. Once the baseline was determined, the process of generating a chemical pattern representative of the field trial was begun.

Visual comparison of the computer-generated plots between the baseline and the experimental contours proved to be the most useful tool in determining which NUSSE3 inputs should be varied to better represent the experimental data. One set of NUSSE3 inputs typically varied were those associated with meteorological conditions. For example, if the predicted pattern was not oriented correctly, then the wind direction was varied based on values recorded by DPG. Data reported at several time intervals provided a range in which these parameters could vary. Each variation in parameters was evaluated in relation to the DPG deposition data through the use of MULTI; these variations were referred to as excursions. The results of each excursion were evaluated using visual inspection and quantitative information. This process was continued until the best predicted to experimental comparison (best-fit) was achieved.

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2. Saucier,R., *NUSSE3 Model Description*, U.S. Army Chemical Research, Development and Engineering Center, Technical Report CRDEC-TR-87046, May 1987 (Unclassified).

3. Saucier, R., *NUSSE3 User's Guide and Reference Manual*, U.S. Army Chemical Research and Development Center, Special Publication CRDC-SP-86009, March 1986 (Unclassified).

The focus of this analysis was to evaluate new quantitative methods applicable to both single and multiple munition field trials. A best-fit criterion was developed based on the results of this analysis.

III. QUANTITATIVE TESTS

Several statistical tests were considered for evaluating chemical munitions. Hypothesis tests chosen for this analysis were the Sign, Mann-Whitney U, and Chi-Square test. The methods used for these tests are those described by Johnson. [4] In addition, a modified version of the Chi-Square was developed; this metric is referred to as the Point-by-Point. Each test was exercised to determine its appropriateness for this application.

1. Sign Test

The nonparametric Sign test is used as a hypothesis test of the median difference of two populations. For this analysis, the null hypothesis (H_0) that was the NUSSE3 model provides a good prediction of the DPG deposition data; in other words, the median difference between the experimental and predicted data was zero. In this analysis the Sign test was applied to the predicted and experimental deposition data at every grid location for a user specified deposition level. For this analysis, deposition levels of $1 mg/m^2$ and greater were examined. The difference between the predicted (NUSSE3) and the experimental (DPG) data was converted to a + or – sign, disregarding the datum if the difference was zero. The number of positive differences and the number of negative differences were summed. The smaller of these sums (s) was selected and used to derive a critical value (s). This value was used to determine whether there was sufficient evidence to reject the H_0 at a certain significance level. The significance level chosen for this analysis was .05: rejection of H_0 when it is actually true.

The determination of the s value is based upon sample size. For sample size n, where $6 \leq n \leq 100$, s is taken from a Critical Value Sign table. If s is less than s, there is not sufficient evidence to reject the H_0, else the H_0 is rejected at the .05 significance level.

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4. Johnson,Robert R., *Elementary Statistics*,Duxbury Press,1976

If n is larger than 100, the Sign test is carried out by means of a normal approximation using a standard normal variable z, where z and x' are defined as follows:

$$z = \frac{\frac{x' - n}{2}}{0.5\sqrt{n}} \qquad (1)$$

$$x' = x + 0.5 \qquad (2)$$

The z value was compared to the range from $-t$ to $+t$, where t was taken from a t distribution table, (two-tailed test) at significance level .05. If z was in the acceptance region, $-t$ to $+t$, there was not sufficient evidence to reject the H_0. If z was in the critical range this indicated a rejection of H_0 at the .05 significance level.

2. Mann-Whitney U Test

The Mann-Whitney U test is a nonparametric hypothesis test for the difference between two independent means. The H_o stated that the mean difference between the experimental and predicted data equals zero. To apply the Mann-Whitney in this analysis, both data sets (predicted and experimental) were placed in ascending order and a rank number assigned to each. If a tie existed, the average rank was assigned to all data involved. The sum of the ranks for the predicted data (S_p) and the sum of the ranks for the experimental data (S_e) were calculated. A U value was calculated with the following formulas:

$$U_p = (n_p)(n_e) + \frac{(n_e)(n_e + 1)}{2} - S_e \qquad (3)$$

$$U_e = (n_p)(n_e) + \frac{(n_p)(n_p + 1)}{2} - S_p \qquad (4)$$

where n_e and n_p were the sample sizes for the experimental and the predicted, respectively. If both sample sizes are less than or equal to 10, the smaller of the U statistic is compared to a critical value (z) taken from the Mann-Whitney table of critical values. The values n_p and n_e must be greater than 1 and the combined sum of n_e and n_p equal to ten in order to use this test. If U is smaller than z there is not sufficient evidence to reject H_o; otherwise, H_o is rejected at the .05 significance level.

If either sample size was larger than twenty or both were larger than ten, the critical value was found through the standard normal variable z:

$$z = \frac{(U - \mu_U)}{\sigma_U} \qquad (5)$$

where U was the smaller of U_e and U_p, μ_U was the mean of the sample sizes, and

σ_U was the standard deviation of the sample sizes. The critical z was compared to the range from $-t$ to $+t$ (two-tailed test) at significance level .05 from the t distribution table. If z was in the acceptance region, there was not sufficient evidence to reject the H_0; z in the critical range rejects H_0 at the .05 significance level.

3. Chi-Square Test

The Chi-Square test is a hypothesis test with several applications. For this analysis, the test was used to compare frequency of occurrences at various deposition levels. The H_0 was that the NUSSE3 model provides a good prediction of the DPG deposition data. The predicted and the experimental data were binned; the initial size for each bin was 10 units (mg/m^2). A minimum of two bins is required to perform the Chi-Square test. If there were less than 5 occurrences for either the predicted or the experimental then the bin was expanded; these final bin ranges varied from one excursion to another. However, the ranges for the predicted and experimental bins were forced to be equal to allow for comparison (i.e. if bin 1 for the predicted data was 1 to $10mg/m^2$, the same was true for the experimental). Once the occurrences in each bin were counted this formula was applied:

$$\chi^2 = \sum_{i=1}^{N} \frac{(E_i - P_i)^2}{P_i} \qquad (6)$$

P and E were the bin counts for the predicted and experimental, respectively, and N was the number of bins. The critical value z was found in the Chi-Square distribution table. If χ^2 was greater than z then the H_0 was rejected at the .05 significance level.

4. Point-by-Point Test

The quantitative test developed specifically for this analysis was the Point-by-Point; it is a modified version of the Chi-Square.[5] The average at each sample point was considered so that it would be an unbiased comparison between the data sets and the denominator was squared to remove the problem of dimensionality. Consequently, this test evaluated area and geometry as well as deposition.

A predicted/experimental comparison was performed at each grid position for a user specified deposition level for either data set. For this analysis, the $1mg/m^2$ level was chosen. The Point-by-Point metric is determined by the

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5. We wish to thank Ric[illegible]cier of BRL for suggesting this metric.

following equation:

$$z = \frac{1}{N} \sum_{i=1}^{N} \frac{(P_i - E_i)^2}{\left(\frac{P_i + E_i}{2}\right)^2} \qquad (7)$$

P and E were the deposition levels at a particular grid position for the predicted and experimental, respectively, and N was the number of data points in the union of the two samples. The value of z ranged from zero to four, with zero indicating an identical comparison.

IV. RESULTS

Each quantitative test was exercised using data from eleven field trials. In order to evaluate the tests, area coverage and visual inspection were performed at the 1,10,40, and $100 mg/m^2$ deposition levels. The primary depositions of concern for this analysis are the 10 and $40 mg/m^2$ levels with $40 mg/m^2$ having precedence over $10 mg/m^2$. Less consideration was given to the $100 mg/m^2$ level because the test grid was too coarse to accurately portray this contour. The $1 mg/m^2$ was used primarily to show the overall size and shape of the pattern. A best-fit criterion was established based on the evaluation of the test results.

A discussion of the data used to evaluate these tests will aid in understanding the results that are to follow. The predicted data set typically contains more data points than the experimental at the lower deposition levels, $5 mg/m^2$ and less. The average predicted data set was more than twice the size of the experimental at the $1 mg/m^2$. Considering the tests and the way in which they were applied, there was an implicit weighting at the lower deposition levels because of this.

Subsets of the data were used to demonstrate the effect the lower deposition levels had on the test results. The subsets also proved useful for evaluating the data sets. The statistical tests were first applied to the entire data set, $1 mg/m^2$ and greater and then to subsets of the data. Subsets examined were deposition levels $10 mg/m^2$ and greater, $40 mg/m^2$ and greater, and $100 mg/m^2$ and greater, in order to shift the emphasis from those lower levels to the levels of most concern. In most cases, there was insufficient data at the $100 mg/m^2$ for the Sign, Mann-Whitney, and Chi-Square tests; hence, the $100 mg/m^2$ was not considered for these tests.

1. Hypothesis Tests

a. **Sign Test.** With the exception of two cases, the Sign test rejected the H_0 for all model predictions when the entire data set was under consideration. Details of the actual deposition levels was lost as a result of considering just the sign differences. Hence, the Sign test did not provide insight into the predicted to experimental comparison.

For trial N4, the baseline z value, -1.22, fell inside the acceptance region -1.96 to $+1.96$, implying there was not sufficient evidence to reject the H_0, that is, the NUSSE3 model makes a good prediction of the DPG data. Figure A-2 of Appendix A shows the overall pattern for the baseline. (All contours plots can be found in Appendix A. The crosshatched contour represents the experimental data and the unfilled contour the predicted.) The area in which predicted, but no experimental, data exists is comparable to the area where there is experimental, but no predicted data. Also, the number of + signs is similar to the number of – signs where the patterns overlap. When these conditions exist, the Sign test fails to reject H_0. Little insight was gained by considering only the sign of the difference between the predicted and experimental data.

The above conditions did not exist for the N4 excursion; therefore the z value, -2.73, was within the critical range and the H_0 was rejected. Inspection of Figures A-2 through A-7, representing the baseline and an excursion contours at 1,10,and40mg/m^2 levels, indicates that the excursion provided a better comparison than the baseline; however, the results of the Sign test did not support this conclusion.

Trial A1 also illustrates why the results of the Sign test were not particularly useful for the best-fit criterion. For the baseline, the z value was -6.00 which was within the critical range. The excursion z was also within the critical range, but by a smaller margin, -4.03. Thus, the Sign test seems to indicate a better comparison for the excursion even though it was still rejected. Visual inspection of the baseline and excursion contours at 1, 10, and $40mg/m^2$, Figures A-8 through A-13, indicate that the excursion was a better fit. Since the H_0 was rejected for both cases, test conclusions were unclear for these baseline and excursion comparisons.

As shown in the analysis of Trial N4, the Sign test lost the detail of the actual deposition values. In general, the results obtained from the Sign test did not provide insight into which set of NUSSE3 parameters gave the "best" representation of the field trial data. Hence, the Sign test was not considered as part of the best-fit criterion.

b. **Mann-Whitney U Test.** The Mann-Whitney test rejected the H_0 for all trials when the entire data was examined. Rejection by the Mann-Whitney test is caused by a large delta in the U_e and the U_p. As the difference in the U statistics increases, the difference between U and the mean also increases. Upon examination of equation 5, as U (the smaller of U_e and U_p) decreases, the absolute value of the z value increases driving it further from the acceptance region (-1.96 to $+1.96$). What causes U_e and U_p to grow apart is a disproportionate change in the sample sizes (n_e and n_p) as compared to the rank values (S_e and S_p). The predicted data set typically contained more data points at the lower deposition levels. It was this clustering of the data points which caused the disproportional change, resulting in rejection. Comparison of the patterns at the higher levels of interest may be good, but the large difference in the number of data points at $1 mg/m^2$ could cause rejection.

Trial N4 provided a good example of the problem with applying the Mann-Whitney to the entire data set. The smallest difference between the baseline and excursion z values for all trials occurred in N4. The Mann-Whitney z value only went from -6.56 to -6.13 as the NUSSE3 parameters were varied; that is, the excursion was only slightly closer to the acceptance region. However, when viewing Figures A-2 through A-7, a drastic improvement in the shape of the patterns is noted from baseline to the excursion. The Mann-Whitney z values did not reflect the magnitude of improvement in pattern shape because the sample sizes and the rank values varied proportionally to each other in the baseline and excursion. Therefore, the difference in U_e and U_p for the baseline was very close to the difference in the U_e and U_p for the excursion.

The excursion of N4 appeared to be a relatively good fit (Figures A-5 through A-7) and yet the Mann-Whitney z at -6.13 was well outside the acceptance region. This was attributed to the ratio of n_p to n_e being 1.05, whereas the ratio of S_p to S_e was 0.68. Since these values were not proportionate, the significant difference in U_p and U_e drove z into the critical range.

Due to the ranking of the data for the Mann-Whitney test and the nature of these data sets the Mann-Whitney test did not give results decisive enough for the best-fit criterion. Therefore, the Mann-Whitney U test was not appropriate as a best-fit criterion.

c. **Chi-Square Test.** The Chi-Square test, which evaluated frequency of occurrences at various deposition levels by binning the data sets, rejected the H_0 for all cases. A NUSSE3 predicted pattern typically has a larger area coverage than the DPG pattern at the lower deposition levels. This can be attributed to many factors, from insufficient data collection to over-simplified simulation of complex phenomena that influence the shape and area of a predicted chemical dissemination pattern. This discrepancy caused rejection of H_0, regardless of the goodness-of-fit at higher deposition levels.

The Chi-Square test was not able to evaluate shape for the chemical pattern; this was attributed to binning the data. By binning the data, only deposition levels are recorded and not location. Without the relative placement of each datum, shape cannot be determined. However, the Chi-Square was able to distinguish a change in area; again, this is due to binning the data. Since frequency of occurrence for each deposition level is determined, area can be evaluated.

For trial N4, the χ^2 values and the area ratios (predicted to experimental) did not change significantly from baseline to excursion. Listed are the χ^2 values and area ratios at $1 mg/m^2$ for trial N4:

	Baseline	Excursion
χ^2	114.99	111.87
Critical Value	11.1	12.6
Area Ratio	0.8	0.9

Contrary to these results, Figures A-2 and A-5 (baseline and excursion) show a considerable change in the shape of the predicted pattern. Conversely, the χ^2 values and the area ratios changed significantly from baseline to excursion for trial N6. Listed are these values at $1 mg/m^2$ for trial N6:

	Baseline	Excursion
χ^2	288.96	137.96
Critical Value	12.6	11.1
Area Ratio	3.6	2.4

However, Figures A-14 and A-15 show only a small change in shape from the baseline to excursion. Consequently, it appears that area was the only factor which influenced the Chi-Square.

Thus, it was concluded that for this analysis the Chi-Square had two shortcomings. First, more data points existed for the predicted than the experimental at the lower deposition levels. Secondly, due to the binning of the data, shape was not an influential factor, as demonstrated in trials N4 and N6. Based on these conclusions, the results of the Chi-Square test were not considered as a best-fit criterion.

d. **Subset Results.** As previously stated, these hypothesis tests were applied to subsets of the data which shifted the emphasis from the lower deposition levels to other levels of interest. When examining the above hypothesis tests, 34 out of 36 cases resulted in rejection of the H_0 at $1 mg/m^2$ and greater. At the $10 mg/m^2$, 29 out of 36 resulted in rejection, and for $40 mg/m^2$ only 12 resulted in rejection. Thus, as the deposition levels of interest increased, the number of rejections decreased, showing the effect the lower deposition levels have on the test results. However, even though the number of rejections decreases at these levels, these subset results do not give enough information about the patterns to

be considered sufficient as a best-fit criterion.

In conclusion, the Sign, Mann-Whitney and Chi-Square tests were not used in the best-fit criterion because they did not decisively address area, shape or deposition comparisons. However, each test does address certain characteristics about the data set which can provide specific insight to the analyst. The Sign Test evaluates the median difference for all paired data sets conveying whether one data set is larger in overall size or deposition. Due to ranking the predicted and experimental data together, the Mann-Whitney Test can show if clustering of data at specific deposition levels occurs for either data set. The Chi-Square Test gives insight to how the frequency distributions of the predicted and experimental data compare. However, the test results by themselves can be misleading. Therefore, to better understand these results a closer look at the actual data is required. Depending on the specific details needed for the analysis objective, these hypothesis tests can be useful.

2. Point-by-Point Test

The Point-by-Point test proved to be the most useful. This metric was sensitive to changes in the predicted data because it considered area, shape, and deposition. The relationship between the Point-by-Point z values and deposition ratio is shown in Figure 1 where the deposition ratio is P/E or E/P, smallest being the numerator. For each individual trial, the initial NUSSE3 run established a baseline value for the Point-by-Point. Statistical values for subsequent excursion(s) were compared to this baseline value to determine which set of NUSSE3 inputs produced a best-fit.

A change in area and shape for the predicted data was reflected in the Point-by-Point test. For trial N8, as shown in Figures A-34 through A-39, there was a large difference between the predicted pattern from the baseline to the excursion. This was reflected in the significant decrease in the Point-by-Point test from 3.01 for the baseline to 2.28 for the excursion.

The Point-by-Point was even sensitive to subtle changes. Trial A3 is used as an example. Listed are the Point-by-Point values for each A3 excursion at $1 mg/m^2$ and greater:

Baseline	3.01
Excursion1	2.94
Excursion2	2.79
Excursion3	2.71
Excursion4	2.81
Excursion5	2.74

Figures A-16 through A-33 show the baseline and excursions contours. In some cases, the change in shape and area was not visually obvious from one excursion

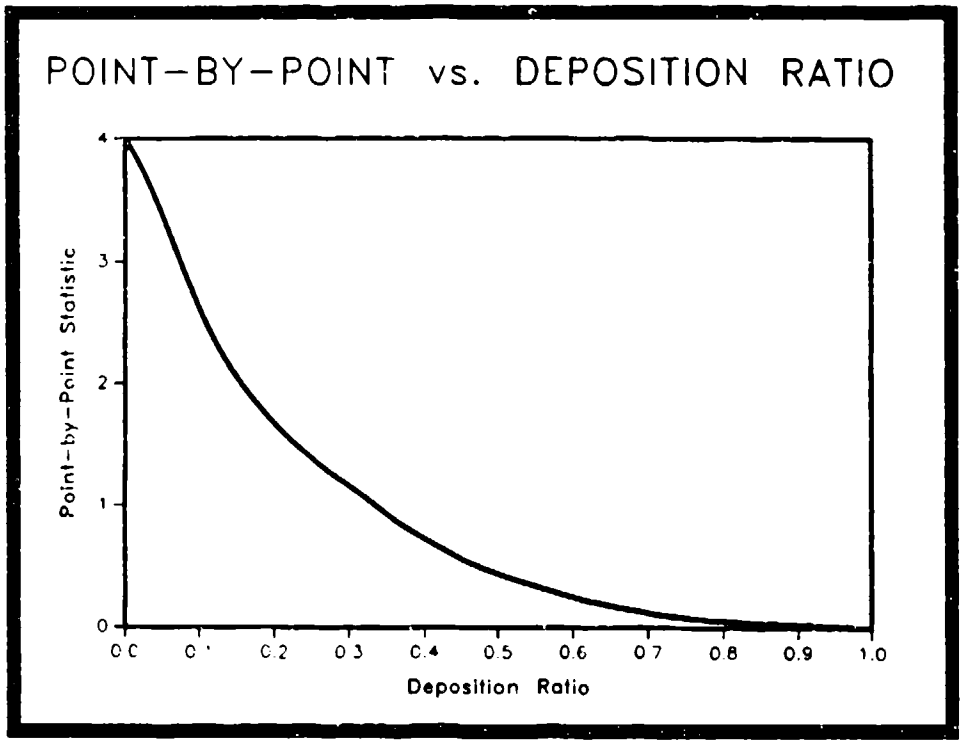

Figure 1. Point-by-Point vs Deposition Ratio

to the next, but the Point-by-Point test was able to make the distinction.

Even when the experimental data was highly discontinuous, as in trial N3, the Point-by-Point still provided insight about the fit. When the entire data set was under consideration, the x values for N3 are 3.23 and 3.32 for the baseline and an excursion, respectively. Figures A-40 through A-45 represent the contours for the baseline and excursion at the 1,10, and $40 mg/m^2$ level. The x values for the baseline and excursion at 1, 10, 40, and $100 mg/m^2$ were as follows:

	1	10	40	100
Baseline	3.23	2.45	2.22	2.30
Excursion	3.32	2.31	2.08	2.13

Upon examination of the contour plots and area coverage ratios, it was determined that the x values accurately portrayed the baseline/excursion comparison at each level. Area coverage ratios of predicted to experimental data are as follows:

	1	10	40	100
Baseline	2.4	0.2	1.8	1.9
Excursion	2.3	0.2	1.8	1.9

Overall the excursion was considered a better fit.

In conclusion, the Point-by-Point metric was the only test considered in determining a best-fit because it included consideration of area, shape, and deposition. Results obtained using the data from the field trials showed that the test was sensitive to changes, substantial or otherwise, in the predicted data. Even for trials where the experimental data was highly irregular, the Point-by-Point metric proved to be useful by examining the results at each deposition level. The Point-by-Point produced results that were consistent with visual inspection for all eleven trials.

V. Supporting Evaluation Methods

As stated throughout this report, visual comparison of the patterns provided a means for evaluating the quantitative tests. The graphical output of the predicted and experimental contours at user specified deposition levels aided in verifying the results of the tests. It was especially useful in comparing the shapes of the patterns. Visual inspection is a tool used to choose NUSSE3 input variations and to portray the information provided by the quantitative tests.

Area coverage was also evaluated by examining the predicted/experimental area ratio. In this analysis, the area ratios for NUSSE3 predictions to experimental data were examined at four deposition levels (1, 10, 40, and $100 mg/m^2$).

Area/deposition (A/D) plots graphically represent area coverage for both predicted and experimental data (examples of A/D plots can be found in Appendix B). Comparison of the predicted to the experimental area coverage at various deposition levels can easily be examined through the area ratios and plots. For example, Trial A3 area ratios are as follows:

	1	10	40	100
Baseline	2.1	1.3	1.6	2.1
Excursion1	2.0	1.3	1.8	2.7
Excursion2	2.0	1.4	1.8	2.8
Excursion3	2.0	1.3	1.8	2.6
Excursion4	2.2	1.5	1.7	1.9
Excursion5	2.2	1.3	1.6	2.2

When evaluating this information, less emphasis was placed on the 1 and $100 mg/m^2$ deposition levels because of the accuracy at which these levels can be measured. Most importantly, the deposition of concern for this analysis was the $40 mg/m^2$ level. (Predicting the area within a 100% error was considered a good prediction.)[6]

Even though the Point-by-Point test includes consideration of area coverage, the area ratios give specific information to better evaluate the NUSSE3 prediction. Visual inspection of the contours was useful in evaluating shape. Therefore, the area coverage ratios and visual inspection will be used in support of the Point-by-Point test to achieve the best-fit.

VI. SUMMARY

Analyzing multiple chemical munitions presented problems that available single munition techniques could not address. To resolve this, the methods were re-examined and new techniques developed that could be applied to both single and multiple munition analyses. Several quantitative tests were considered and tested using field trial data. This methodology is embodied in a computer code called MULTI.

Comparing area, shape and deposition of the chemical patterns was primary in deciding which test would be included in the best-fit criterion. A best-fit criterion was established based on the results obtained from the tests. Only one of the tests addressed all three points: the Point-by-Point. Therefore, the Point-by-

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6. R. Saucier, USABRL, private communication.

Point is the primary metric used to determine a best-fit.

Visual inspection of the contour plots aids in deciding which NUSSE3 inputs to vary, as well as used to achieve a best-fit. The ratios of the area are also examined to ensure these values are within a reasonable (100%) error; primarily at the deposition of interest. The Sign, Mann-Whitney and Chi-Square tests were not appropriate as a best-fit criterion but could provide insight into certain characteristics about the data sets.

For this analysis, consistent results were obtained by use of this criterion. After examining all the tests and the data used in the evaluation, it is concluded that evaluating the quantitative test, visual inspection, and area coverage simultaneously is essential. These tests used in conjunction provide the necessary information to perform a predicted to experimental data analysis of chemical munitions.

REFERENCES

1. Klopcic, J. Terrence and Hindman, Tracy P., *Deposition Modeling and Effectiveness Evaluation Using Chemical Weapon Field Trial Dispersion Data*, U.S. Army Ballistic Research Laboratory, Technical Report BRL-MR-3652, March 1988, (Unclassified).

2. Saucier,R., *NUSSE3 Model Deecription*, U.S. Army Chemical Research, Development and Engineering Center, Technical Report CRDEC-TR-87046, May 1987 (Unclassified).

3. Saucier, R., *NUSSE3 User's Guide and Reference Manual*, U.S. Army Chemical Research and Development Center, Special Publication CRDC-SP-86009, March 1986 (Unclassified).

4. Johnson,Robert R., *Elementary Statistics*,Duxbury Press,1976

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APPENDIX A

Contour Plots

Each plot depicts the experimental and predicted data at a specific deposition level for each trial. The crosshatched area represents the experimental data and the unfilled contour the predicted. Listed are the Figures:

Figure A-1	Dugway Test Grid
Figures A-2 - A-4	Baseline Trial N4
Figures A-5 - A-7	Excursion Trial N4
Figures A-8 - A-10	Baseline Trial A1
Figures A-11 - A-13	Excursion Trial A1
Figure A-14	Baseline Trial N6
Figure A-15	Excursion Trial N6
Figures A-16 - A-18	Baseline Trial A3
Figures A-19 - A-21	Excursion 1 Trial A3
Figures A-22 - A-24	Excursion 2 Trial A3
Figures A-25 - A-27	Excursion 3 Trial A3
Figures A-28 - A-30	Excursion 4 Trial A3
Figures A-31 - A-33	Excursion 5 Trial A3
Figures A-34 - A-36	Baseline Trial N8
Figures A-37 - A-39	Excursion Trial N8
Figures A-40 - A-42	Baseline Trial N3
Figures A-43 - A-45	Excursion Trial N3

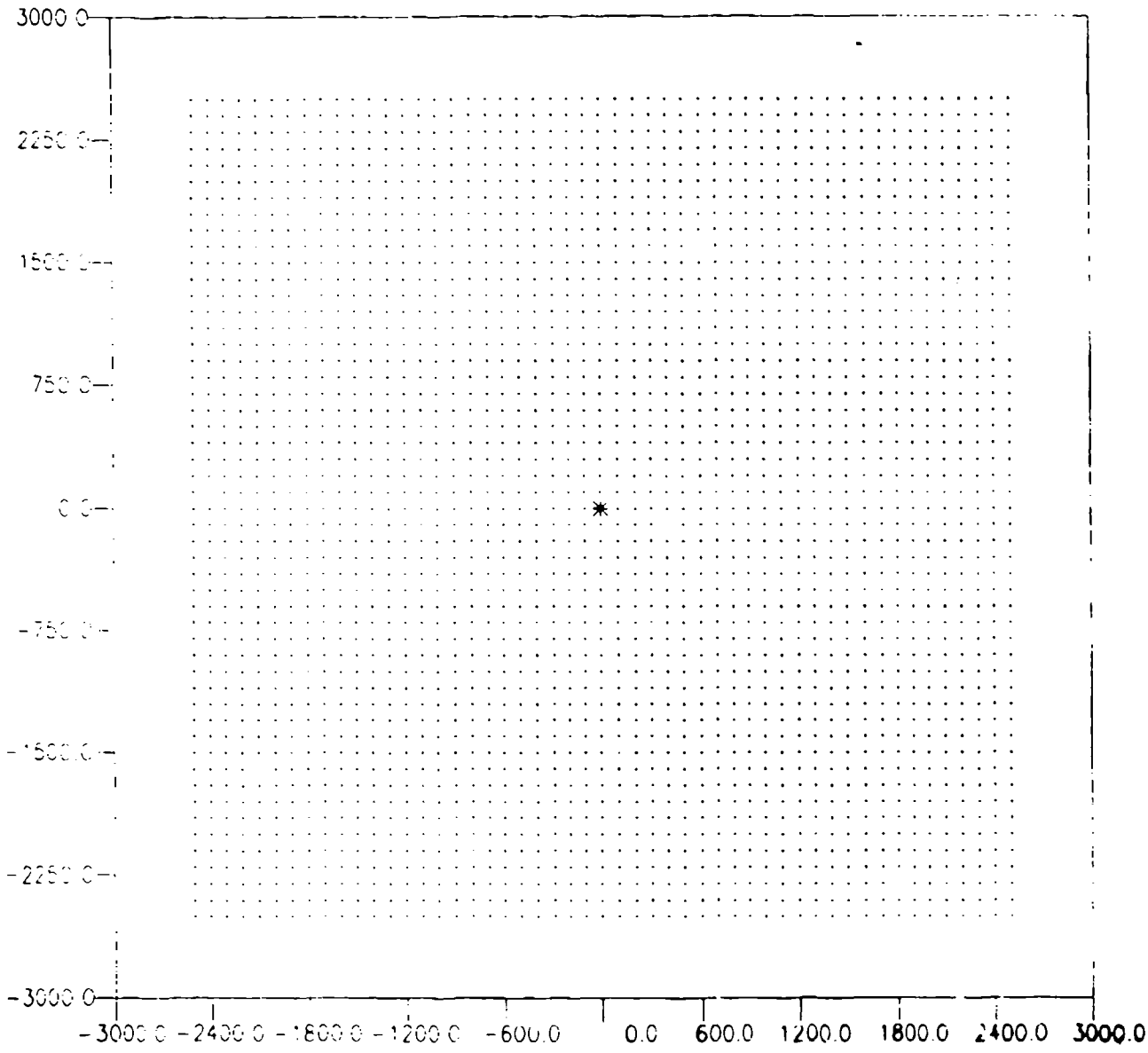

Figure A-1 Dugway Test Grid

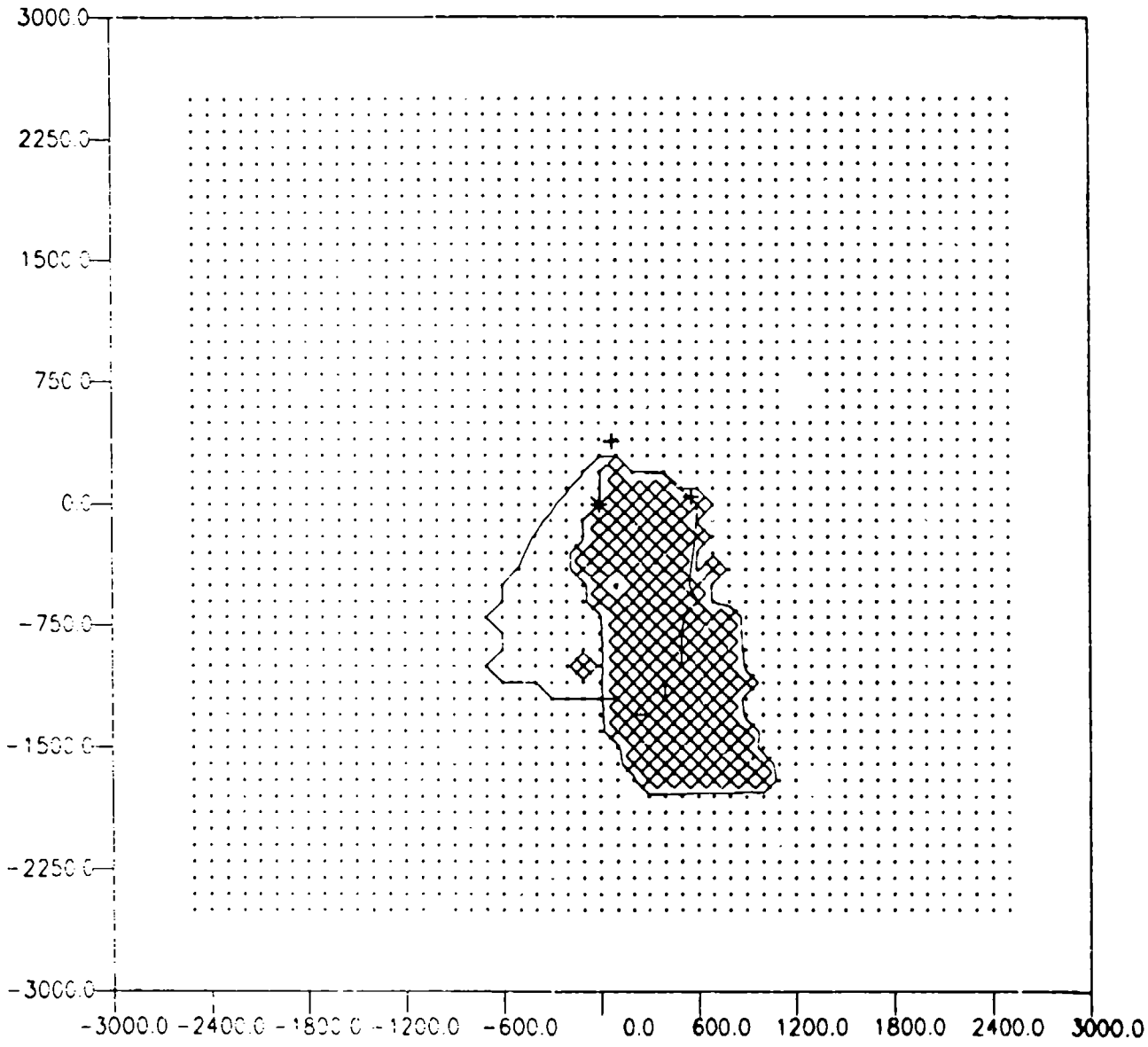

Figure A-2 **Baseline Trial N4, 1 mg/m^2**

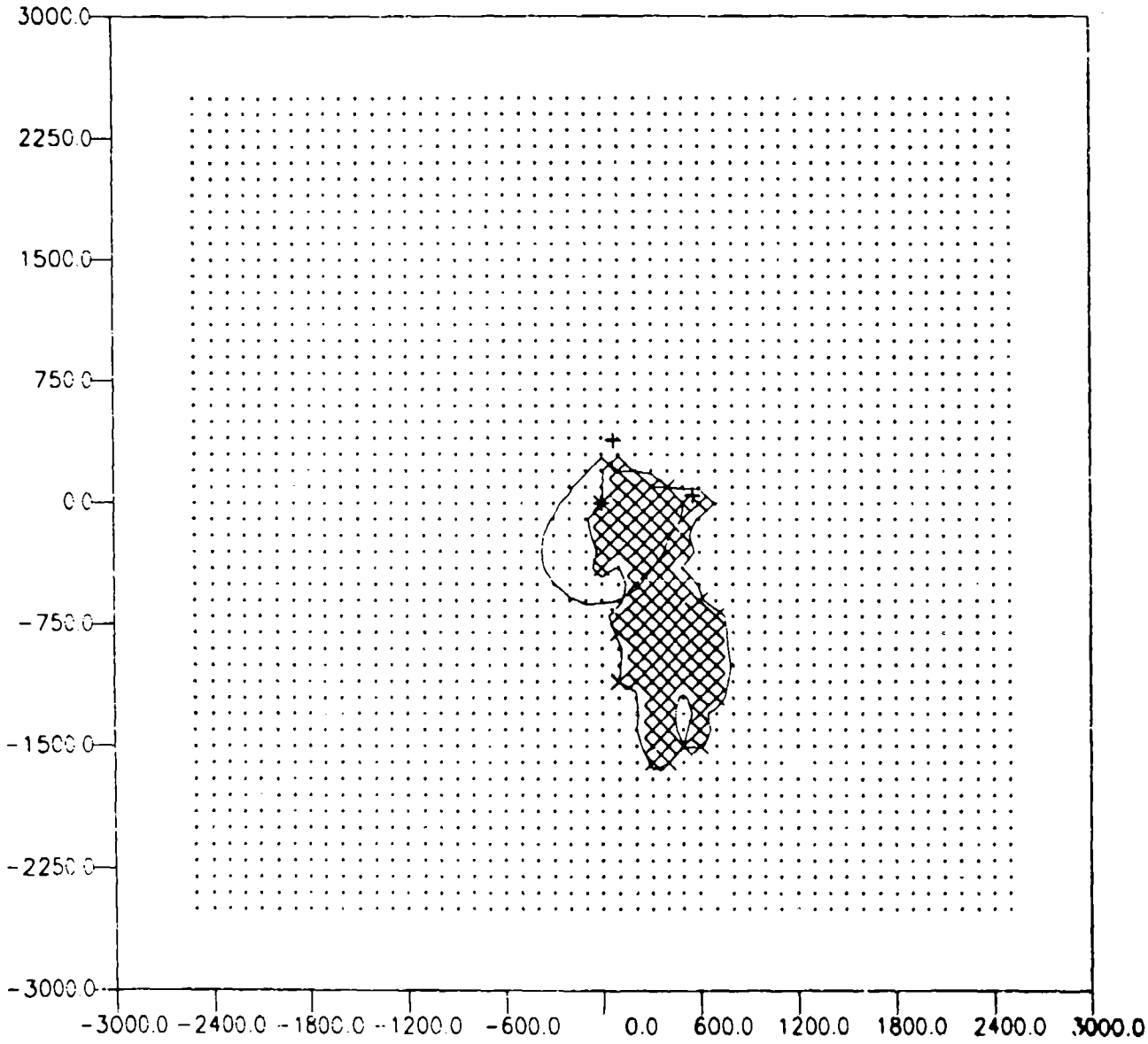

Figure A-3 Baseline Trial N4, 10 mg/m^2

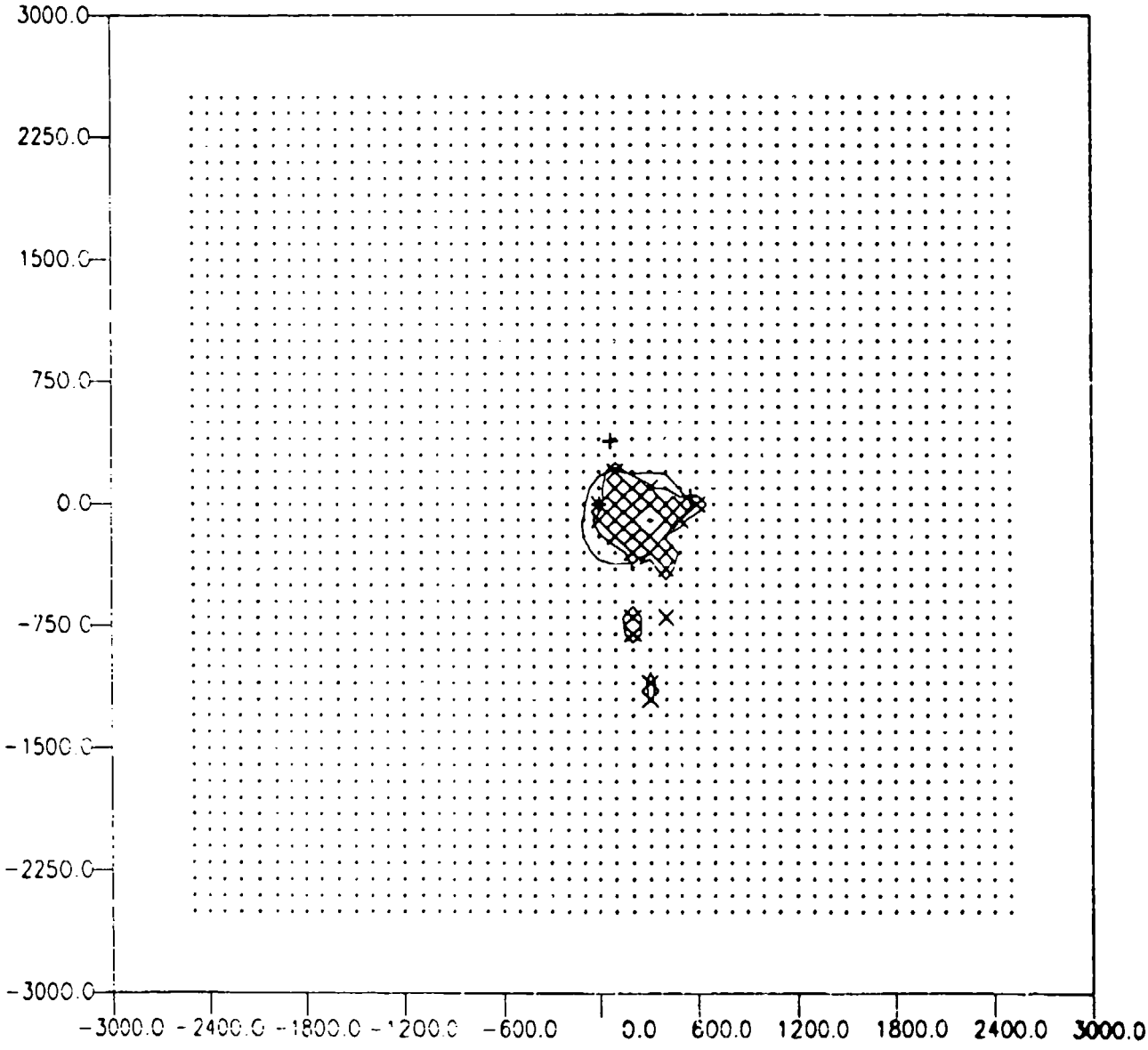

Figure A-4 Baseline Trial N4, 40 mg/m^2

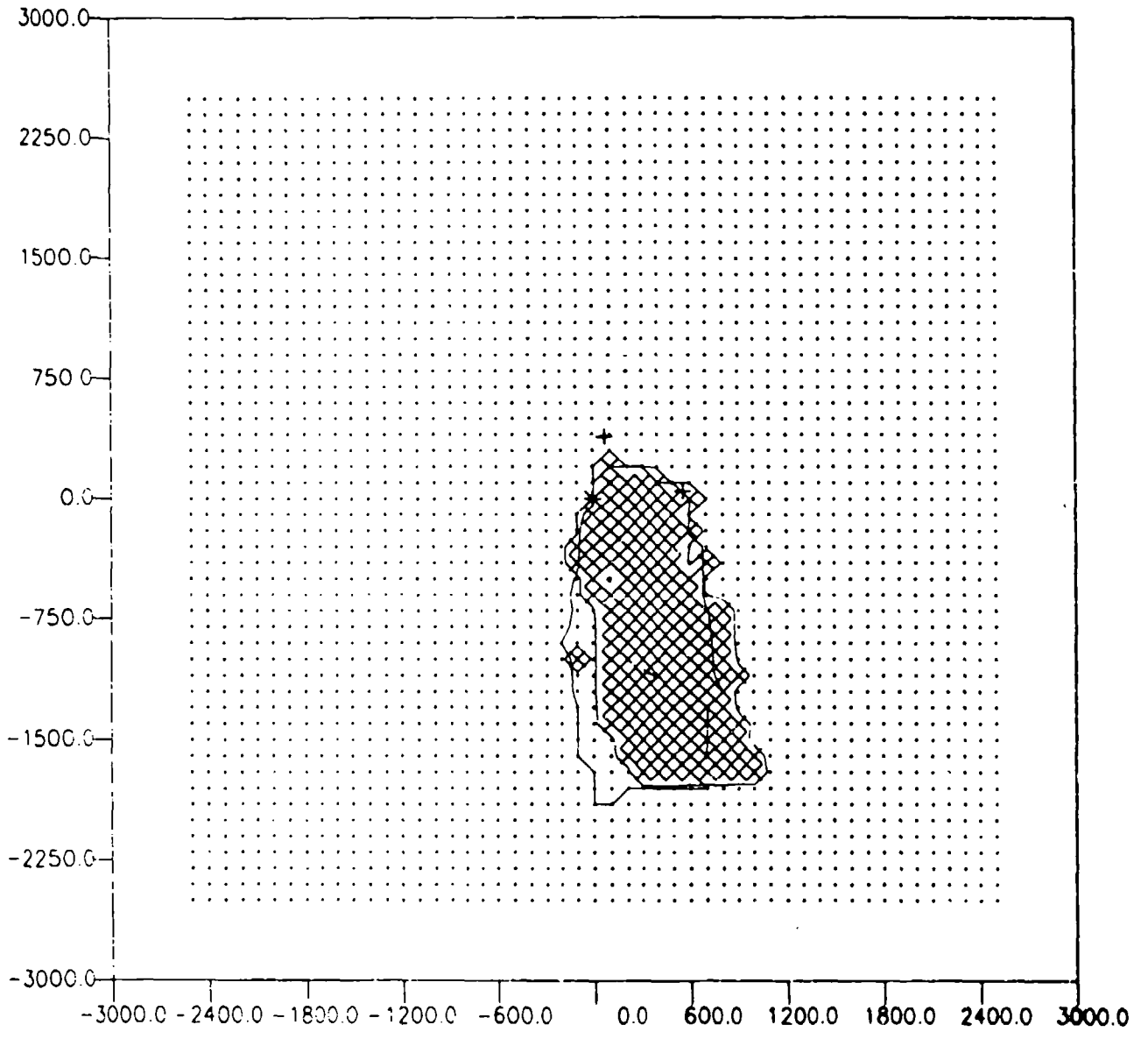

Figure A-5 Excursion Trial N4, 1 mg/m^2

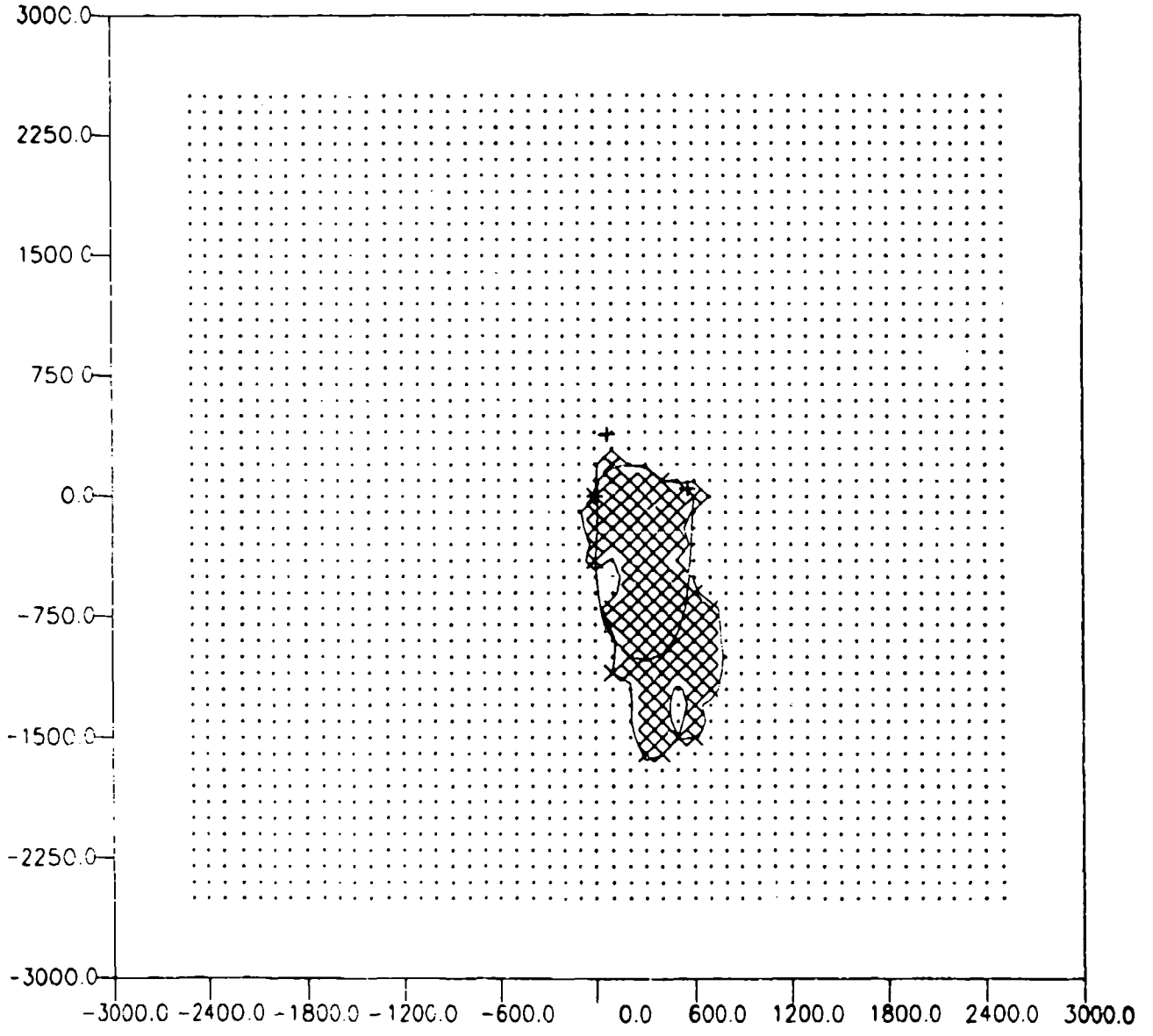

Figure A-6 Excursion Trial N4, 10 mg/m^2

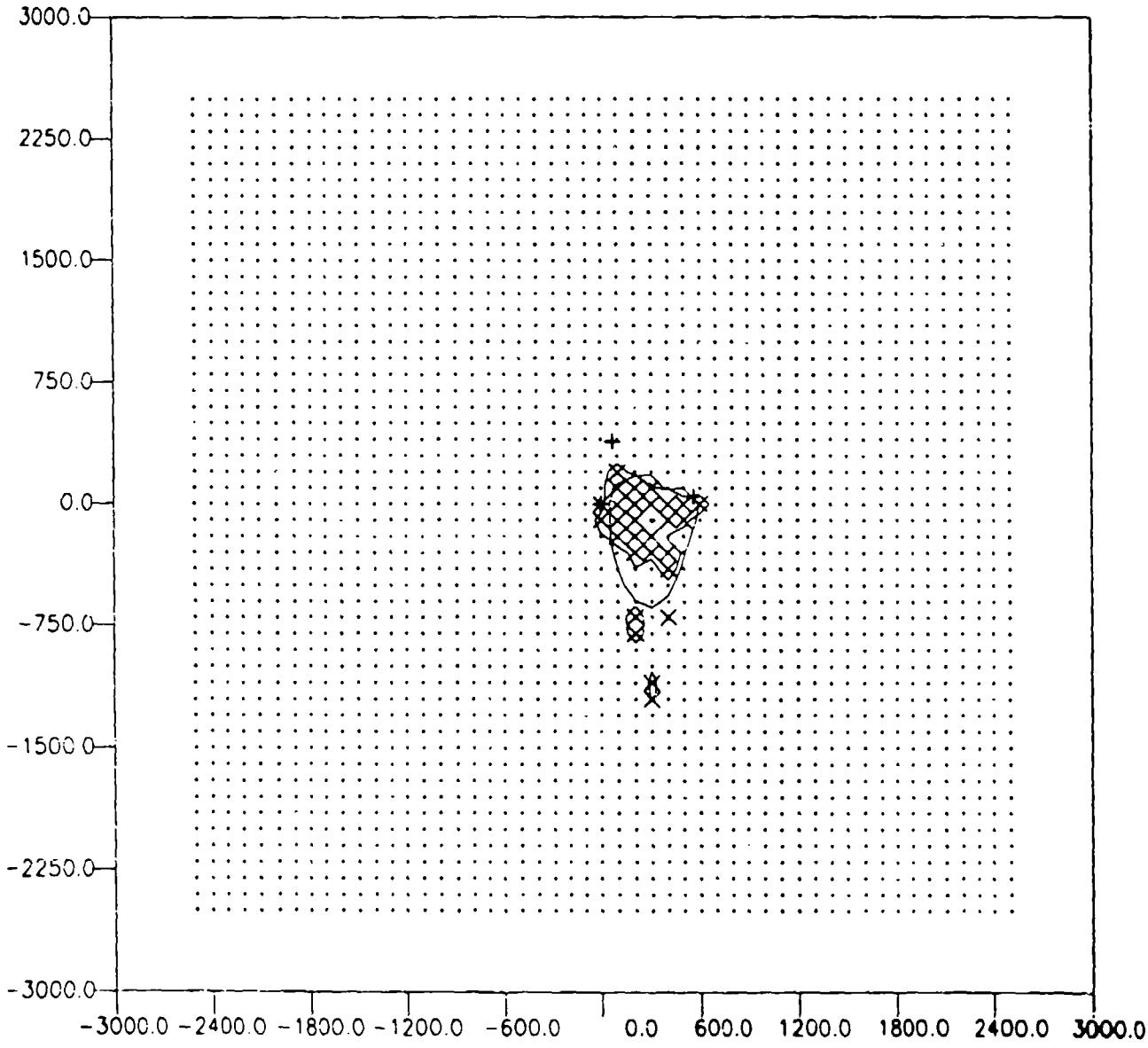

Figure A-7 Excursion Trial N4, 40 mg/m^2

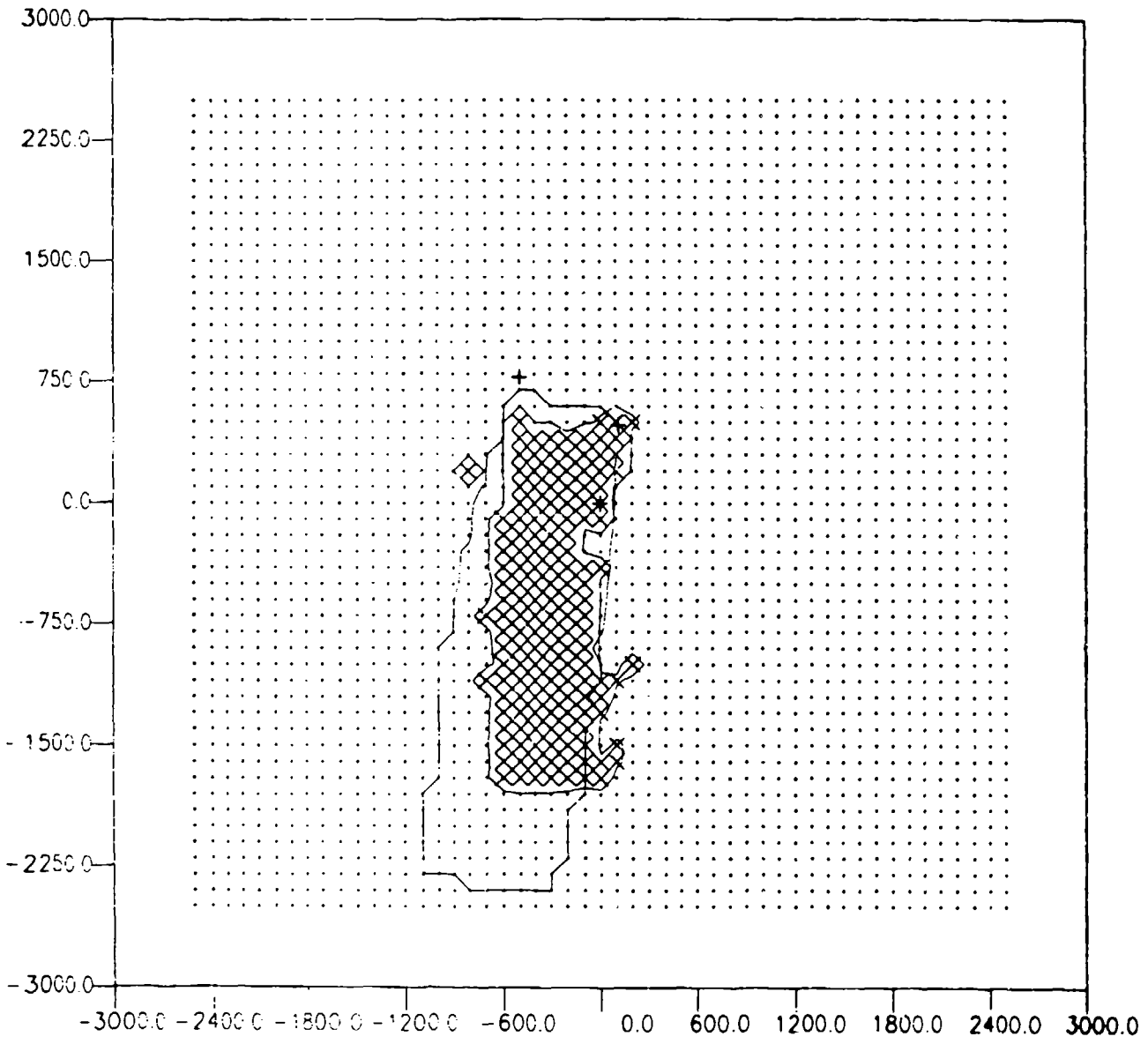

Figure A-8 Baseline Trial A1, 1mg/m^2

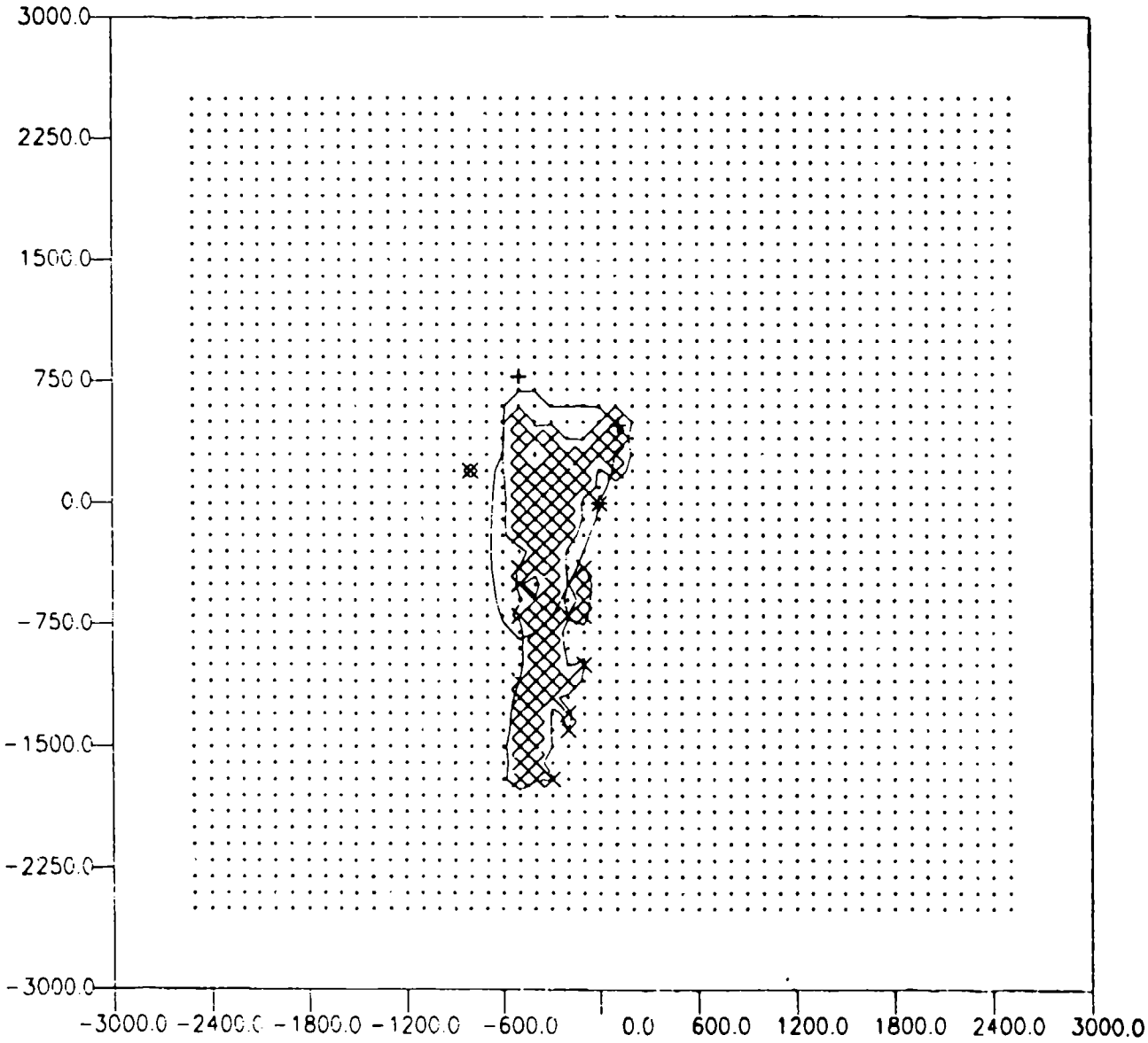

Figure A-9 Baseline Trial A1, 10 mg/m^2

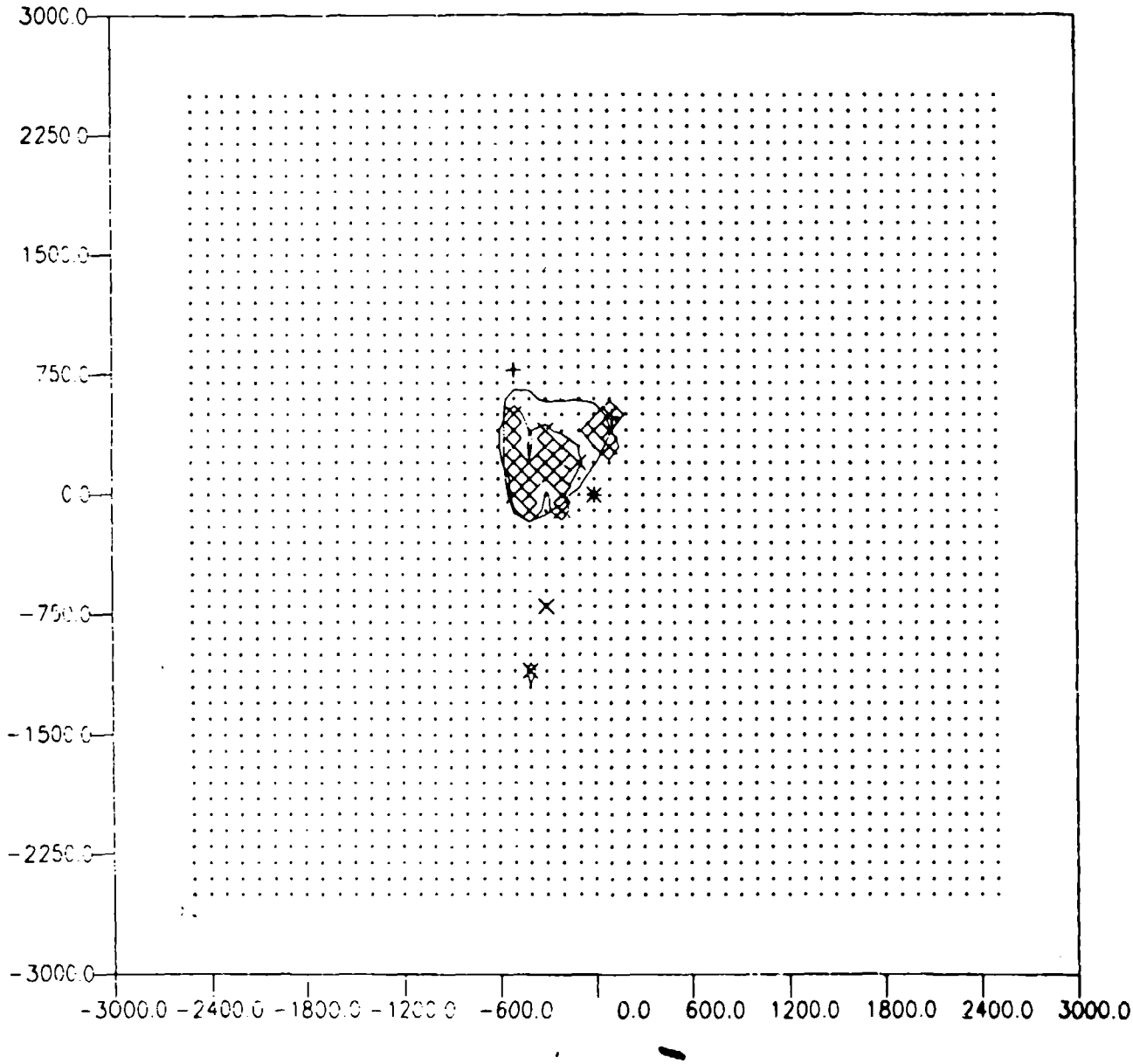

Figure A-10 Baseline Trial A1, 40 mg/m^2

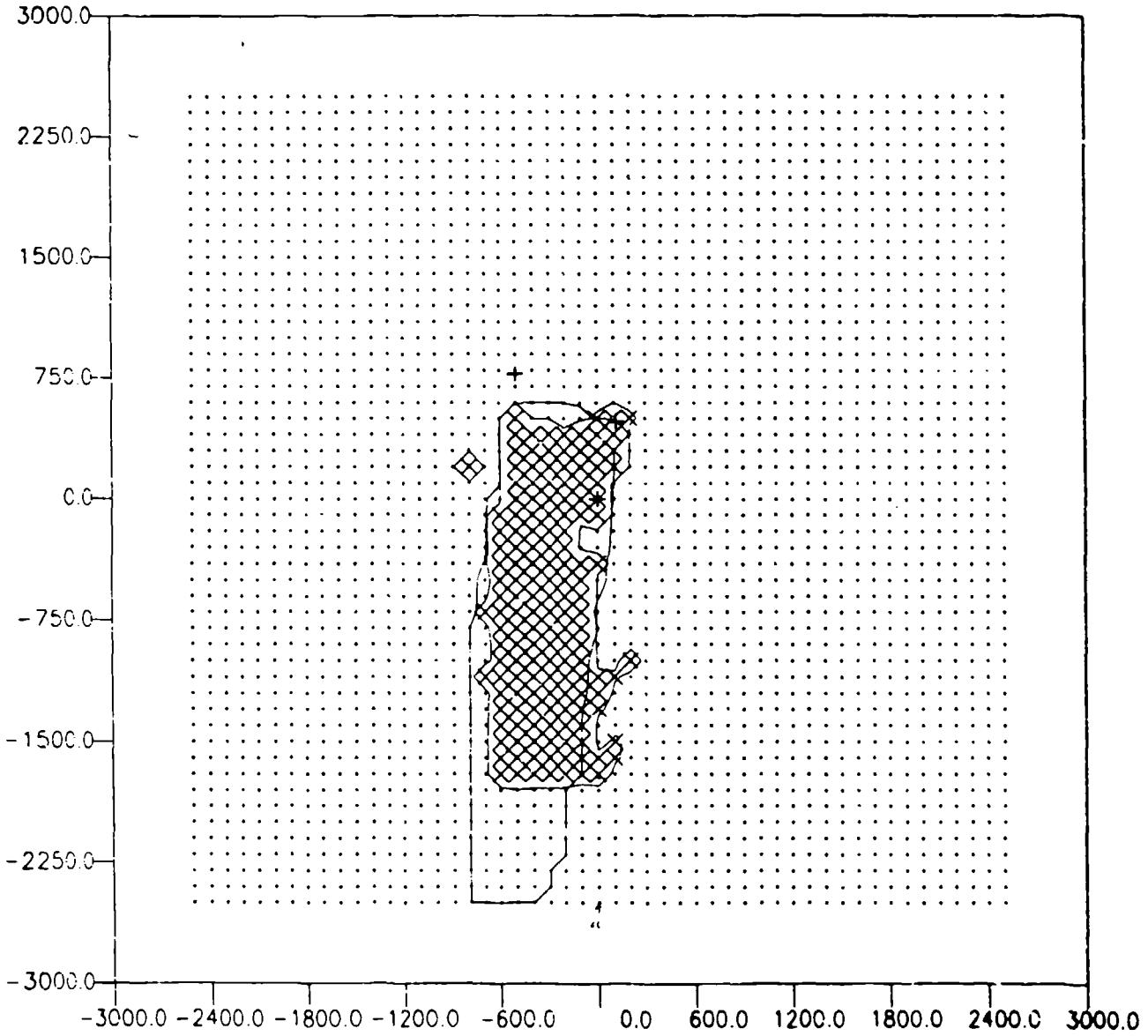

Figure A-11 Excursion Trial A1, 1 mg/m^2

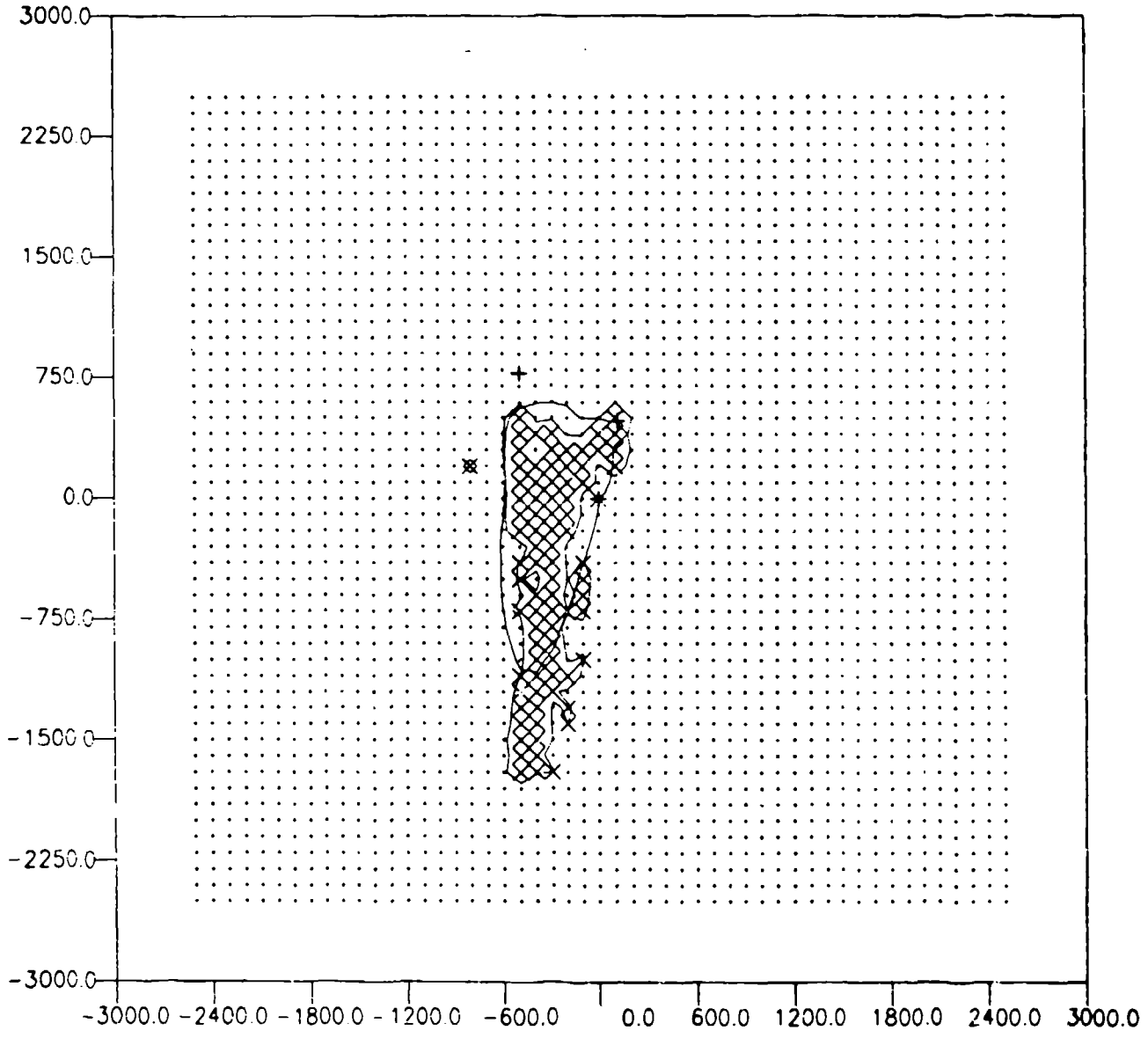

Figure A-12 Excursion Trial A1, 10 mg/m^2

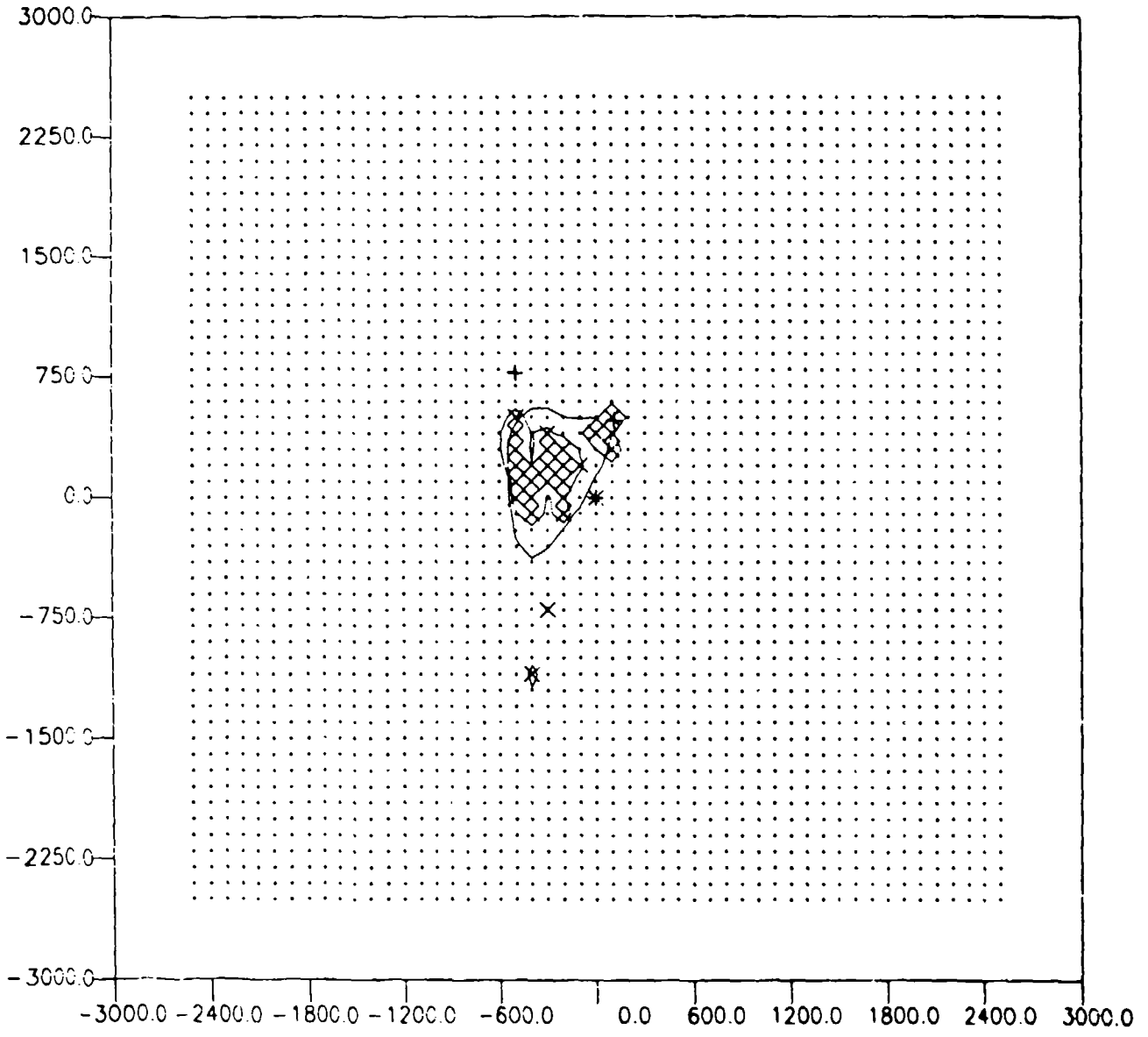

Figure A-13 Excursion Trial A1, 40 mg/m^2

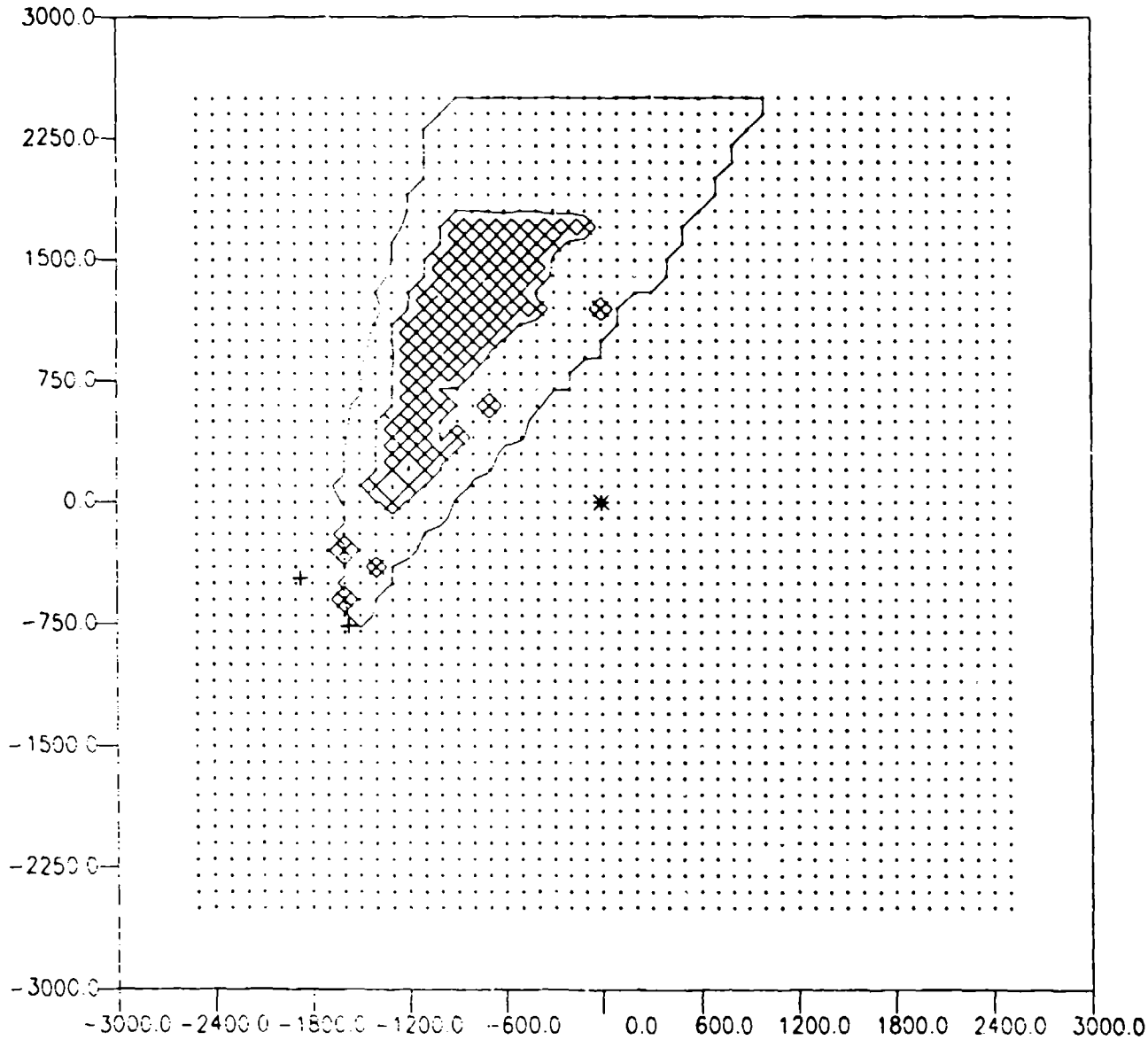

Figure A-14 Baseline Trial N6, 1 mg/m^2

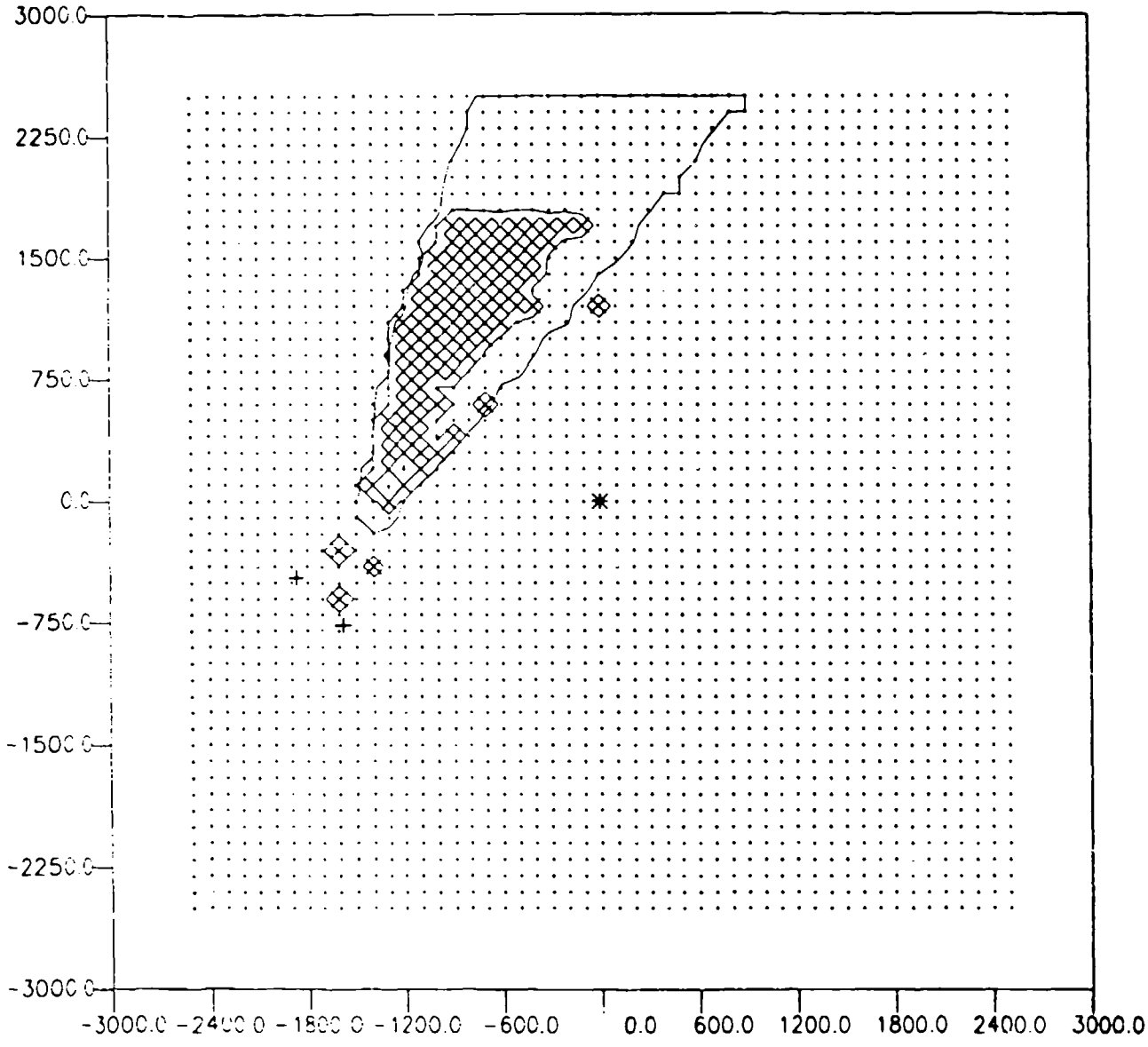

Figure A-15 Excursion 1 Trial N6, 1 mg/m^2

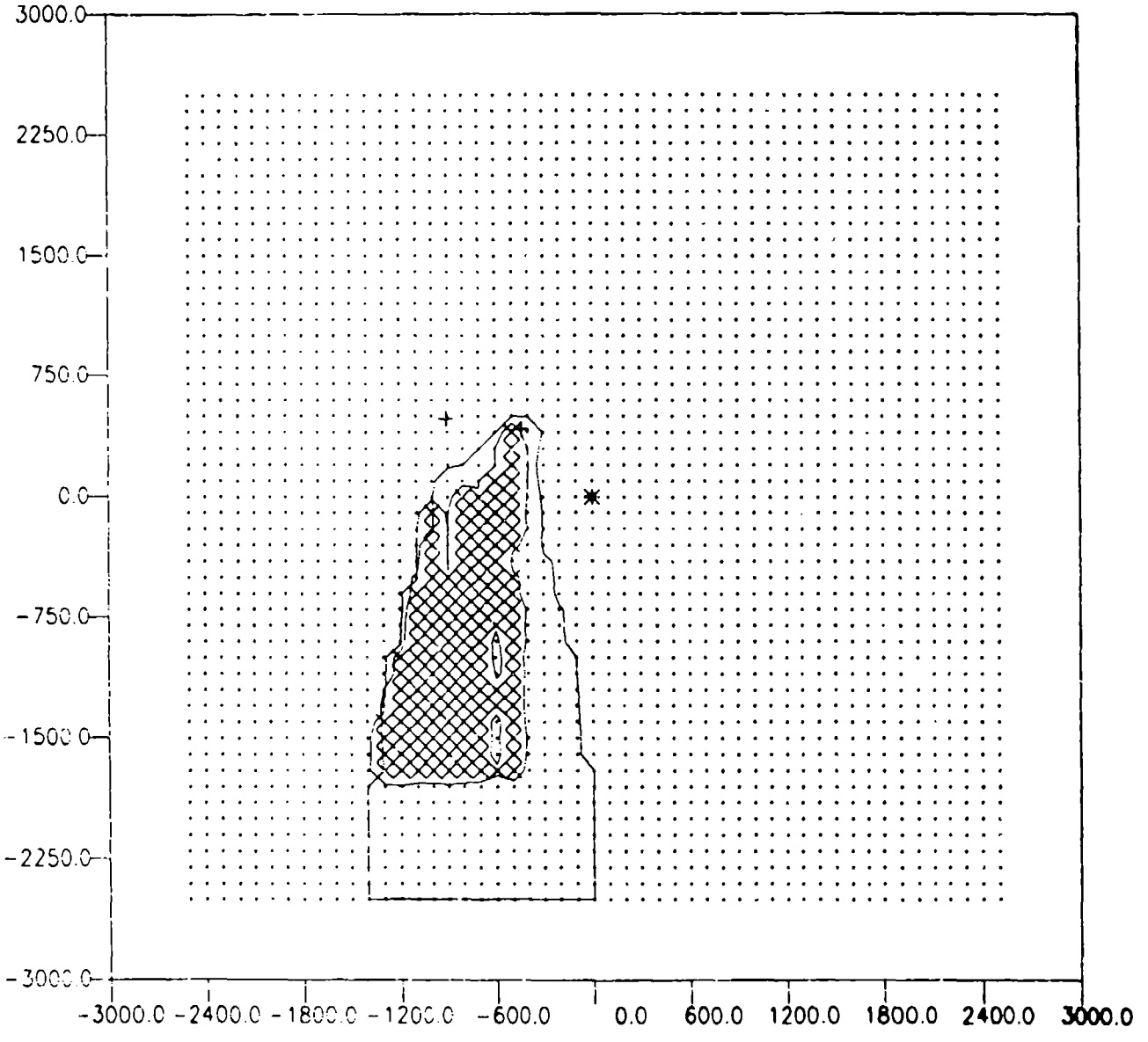

Figure A-16 Baseline Trial A3, 1 mg/m^2

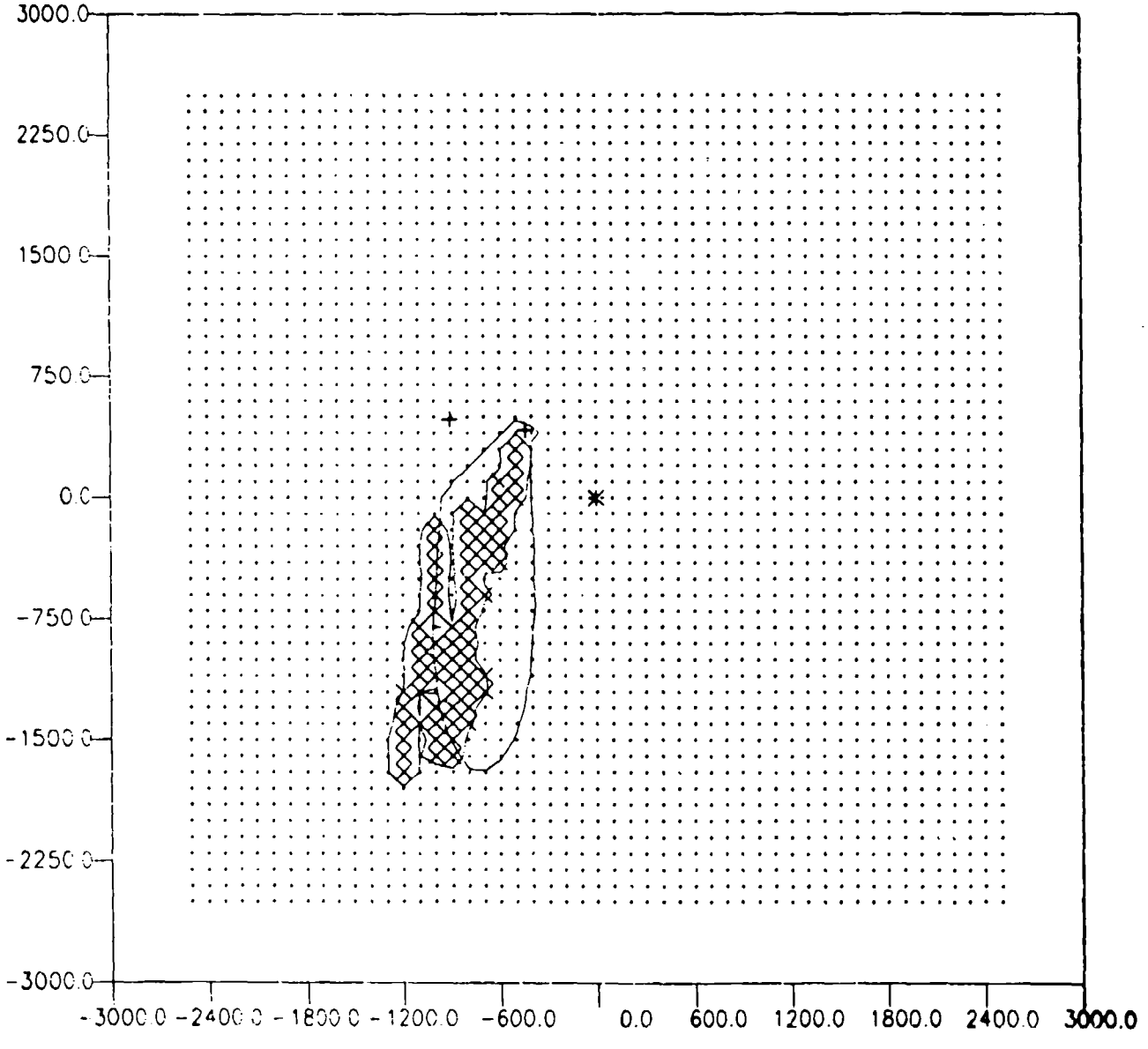

Figure A-17 Baseline Trial A3, 10 mg/m^2

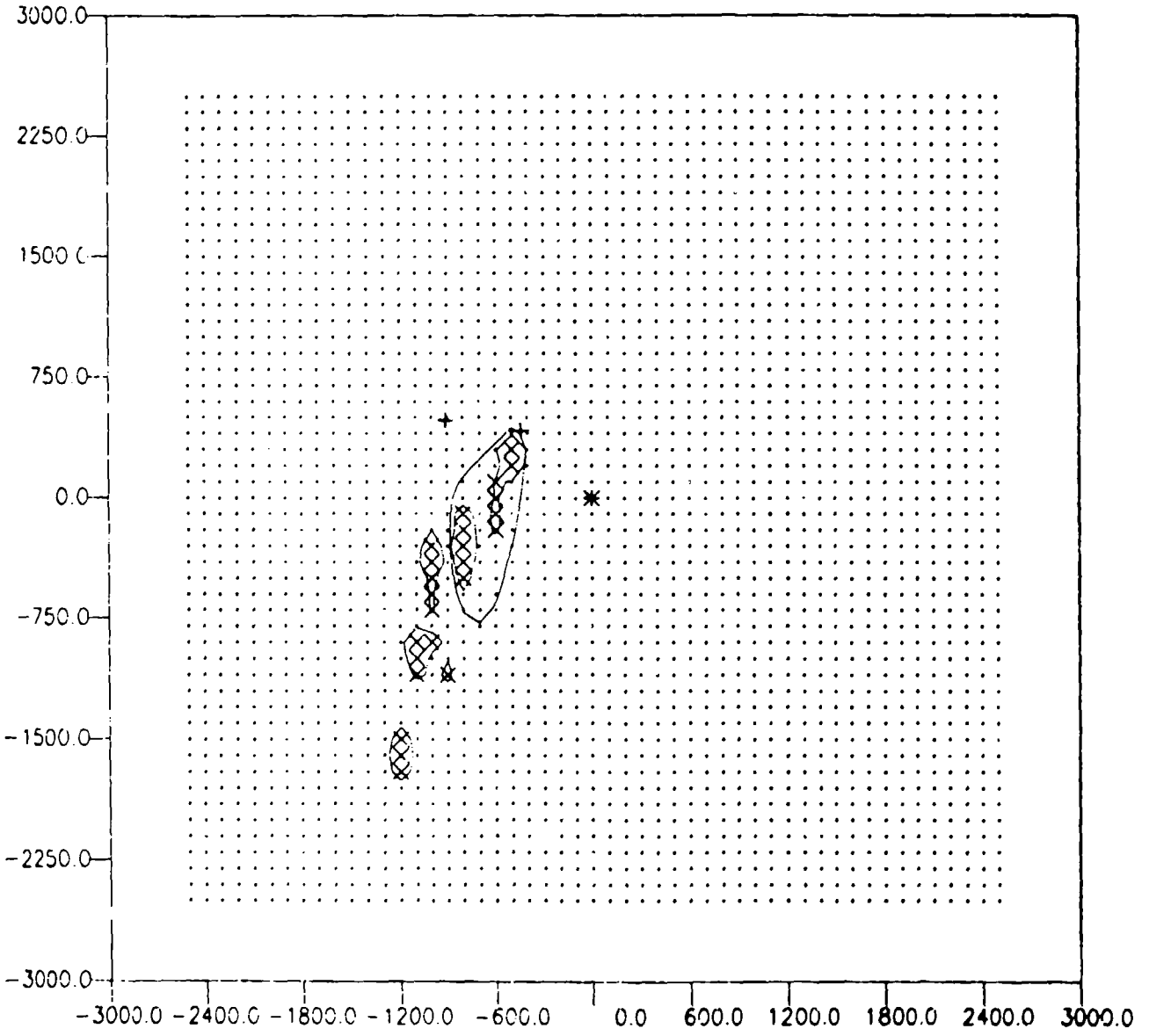

Figure A-18 Baseline Trial A3, 40 mg/m^2

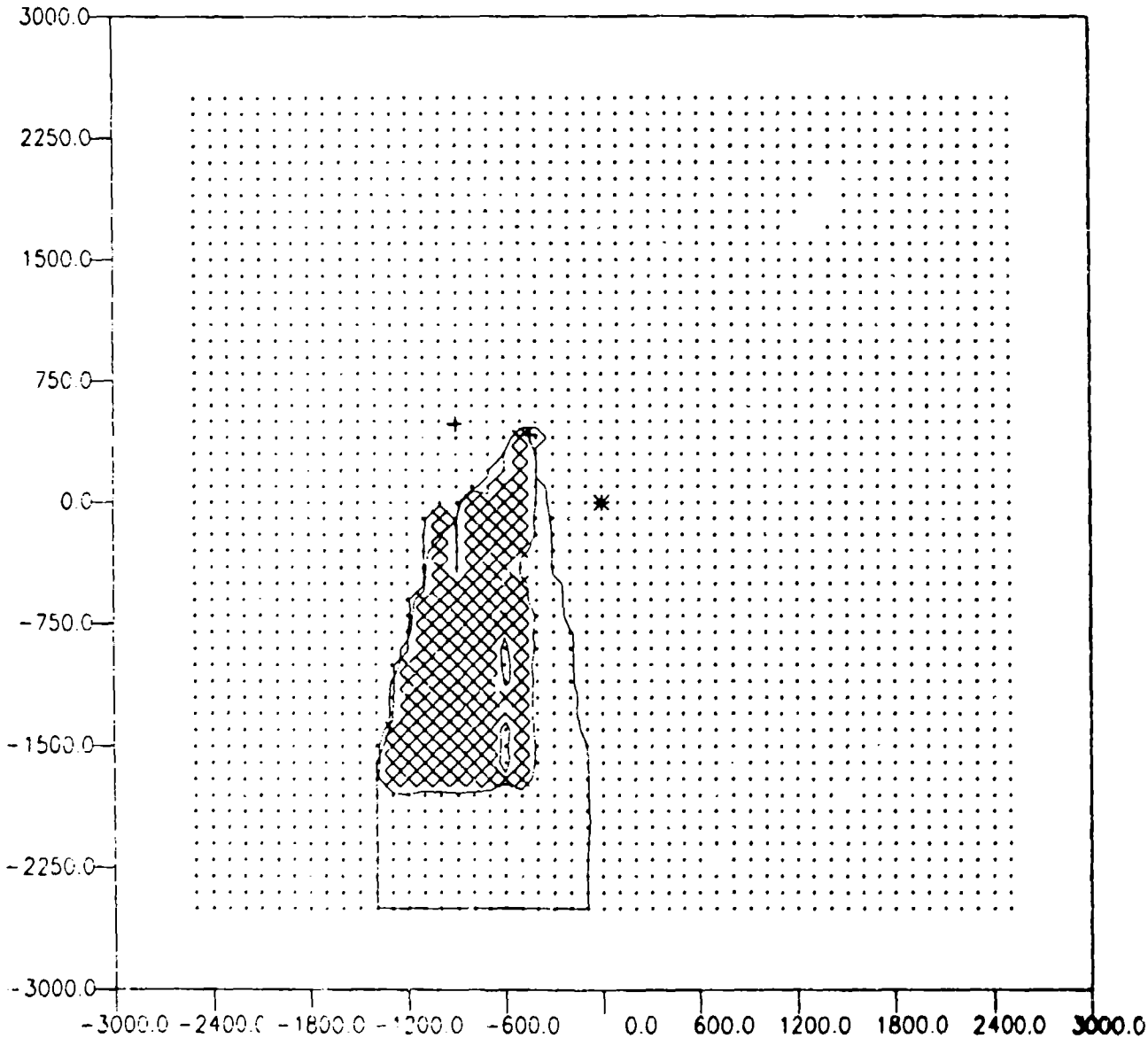

Figure A-19 Excursion 1 Trial A3, 1 mg/m^2

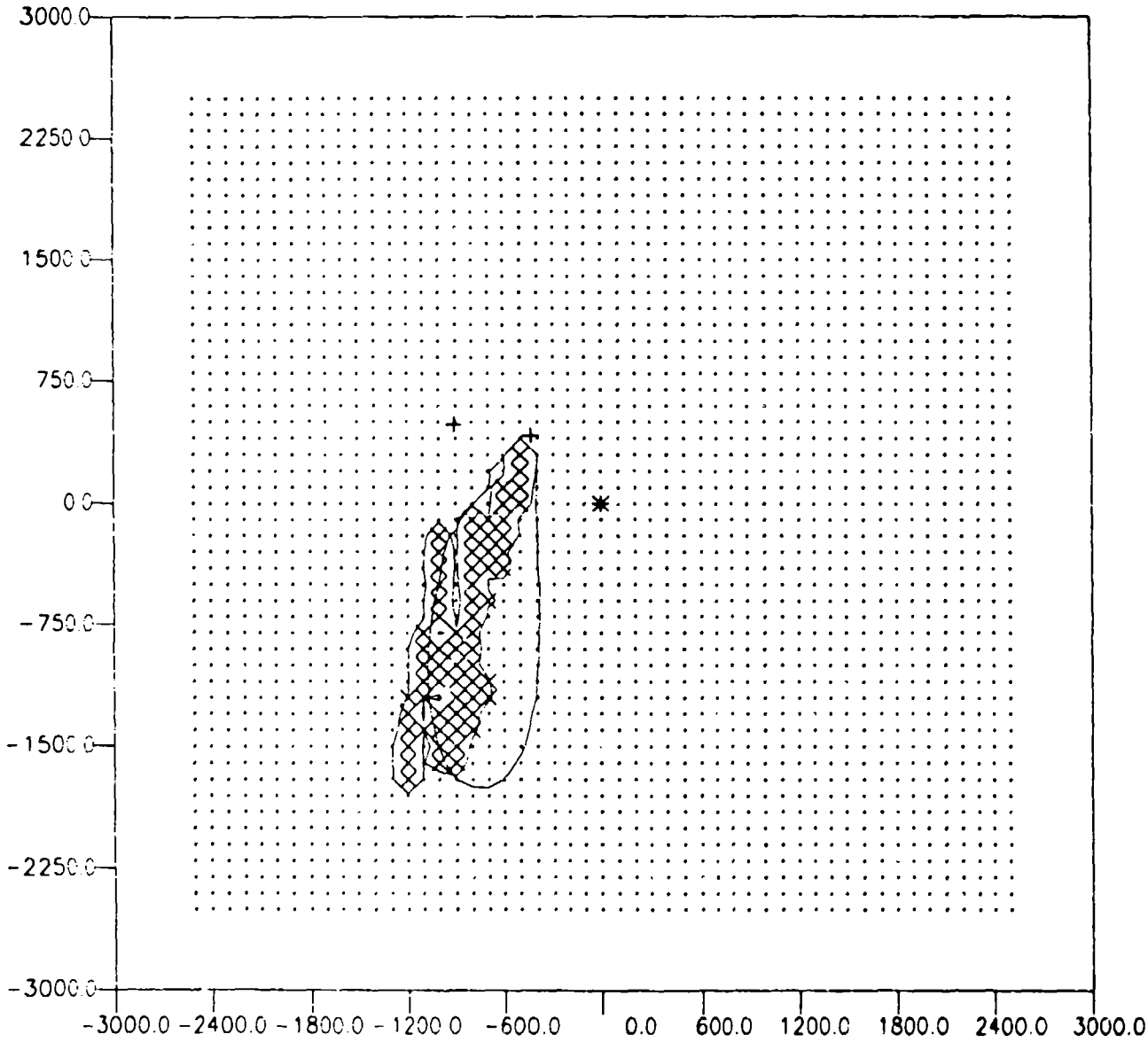

Figure A-20 Excursion 1 Trial A3, 10 mg/m^2

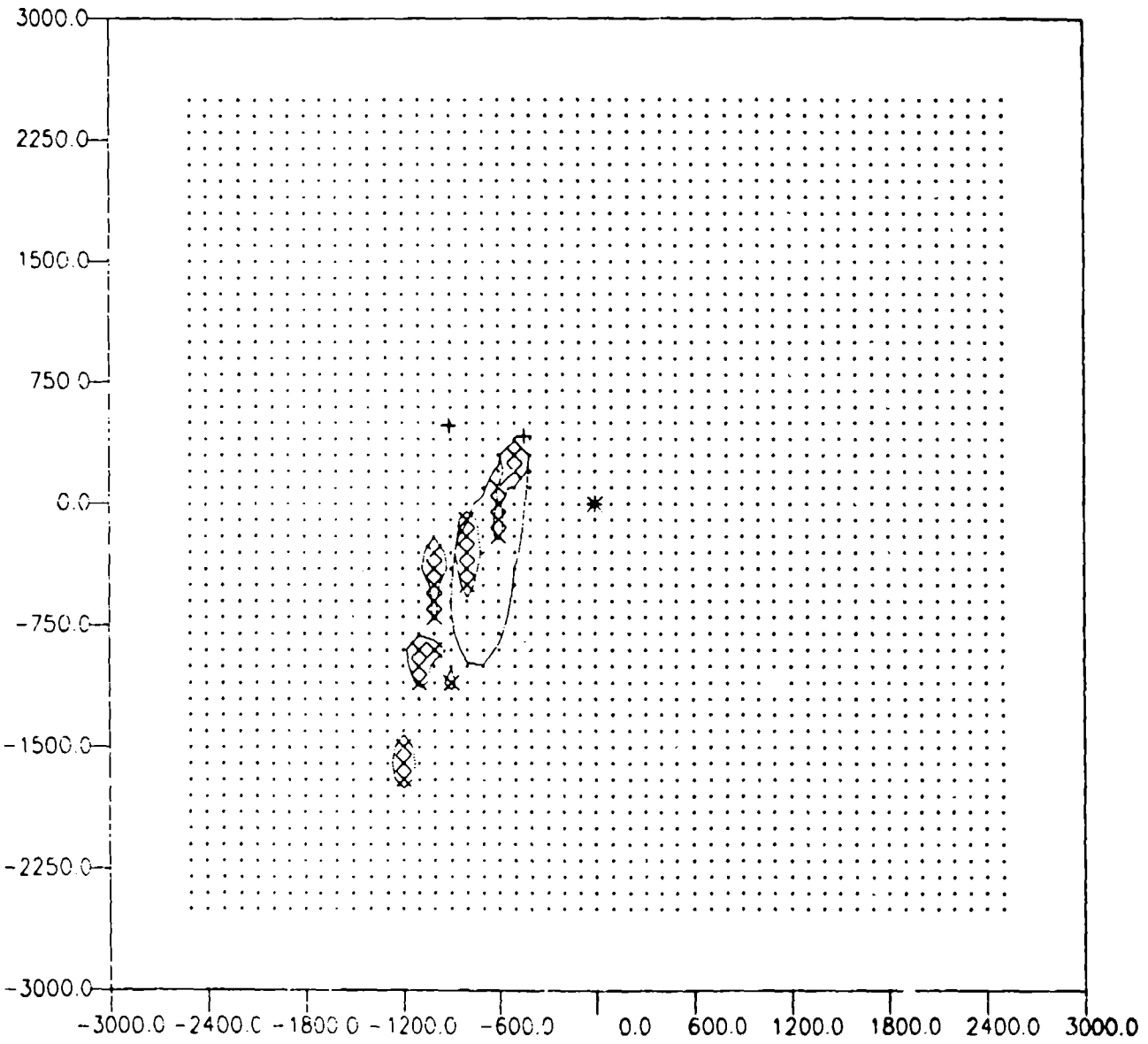

Figure A-21 Excursion 1 Trial A3, 40 mg/m^2

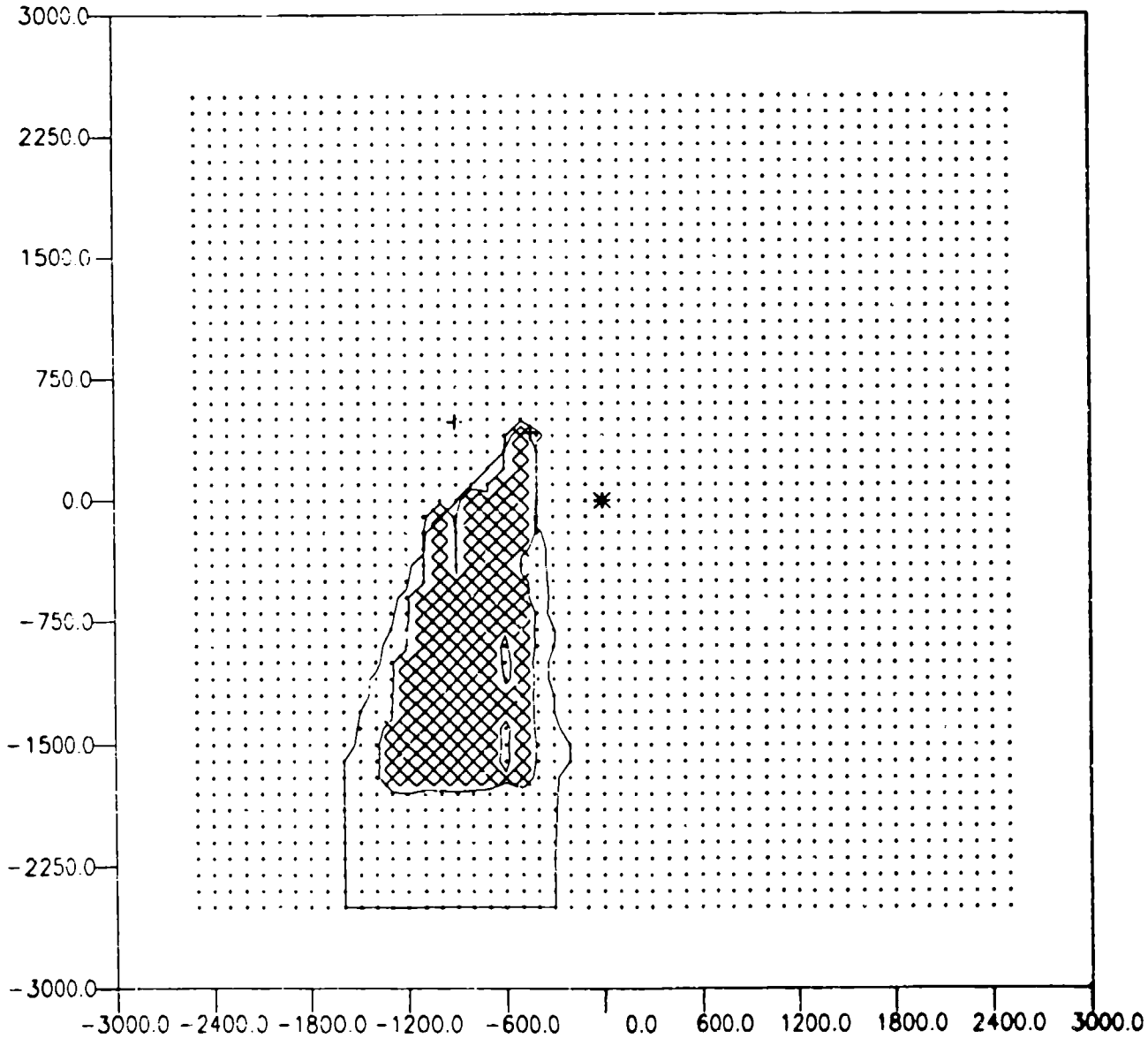

Figure A-22 Excursion 2 Trial A3, 1 mg/m^2

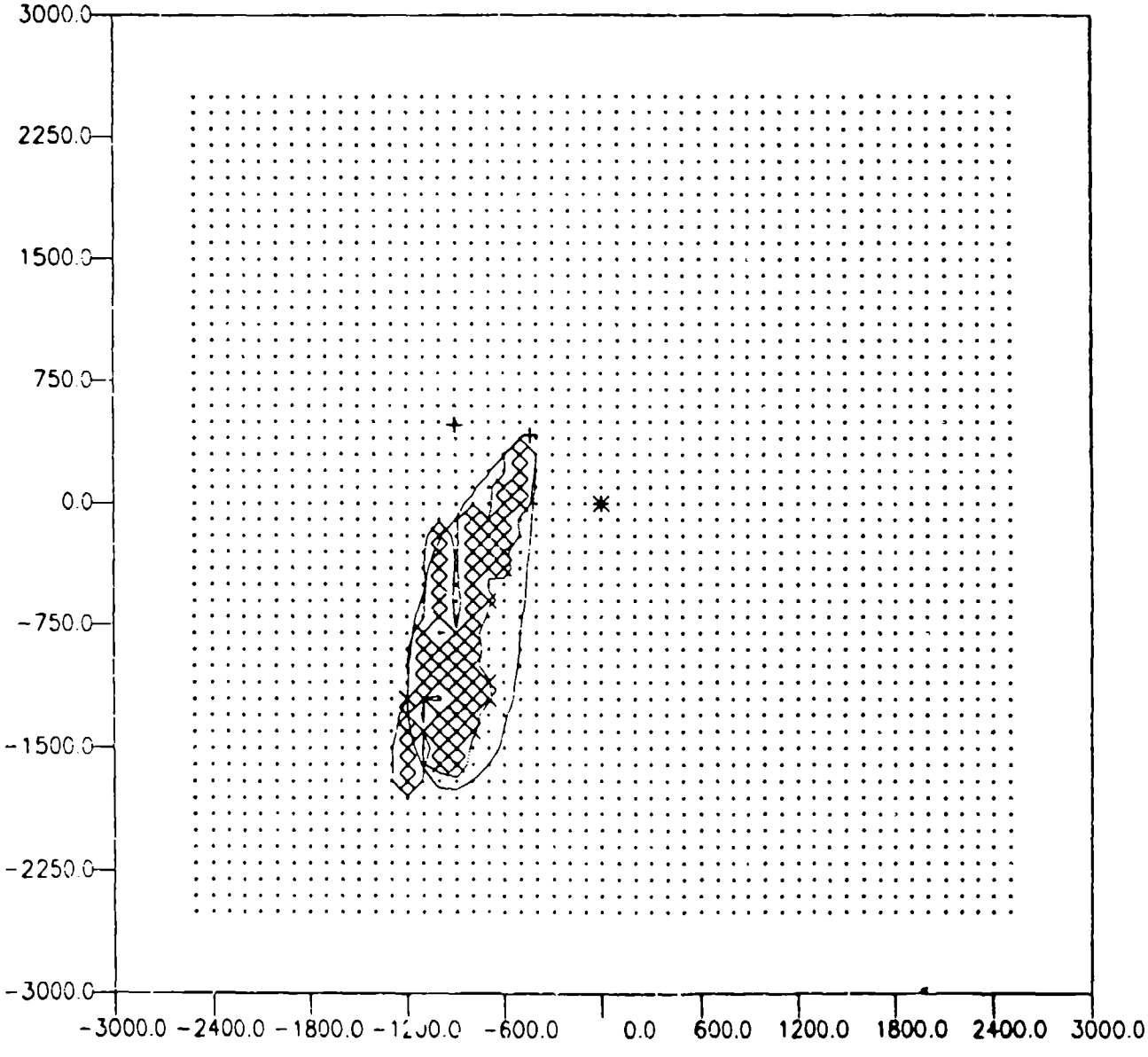

Figure A-23 Excursion 2 Trial A3, 10 mg/m^2

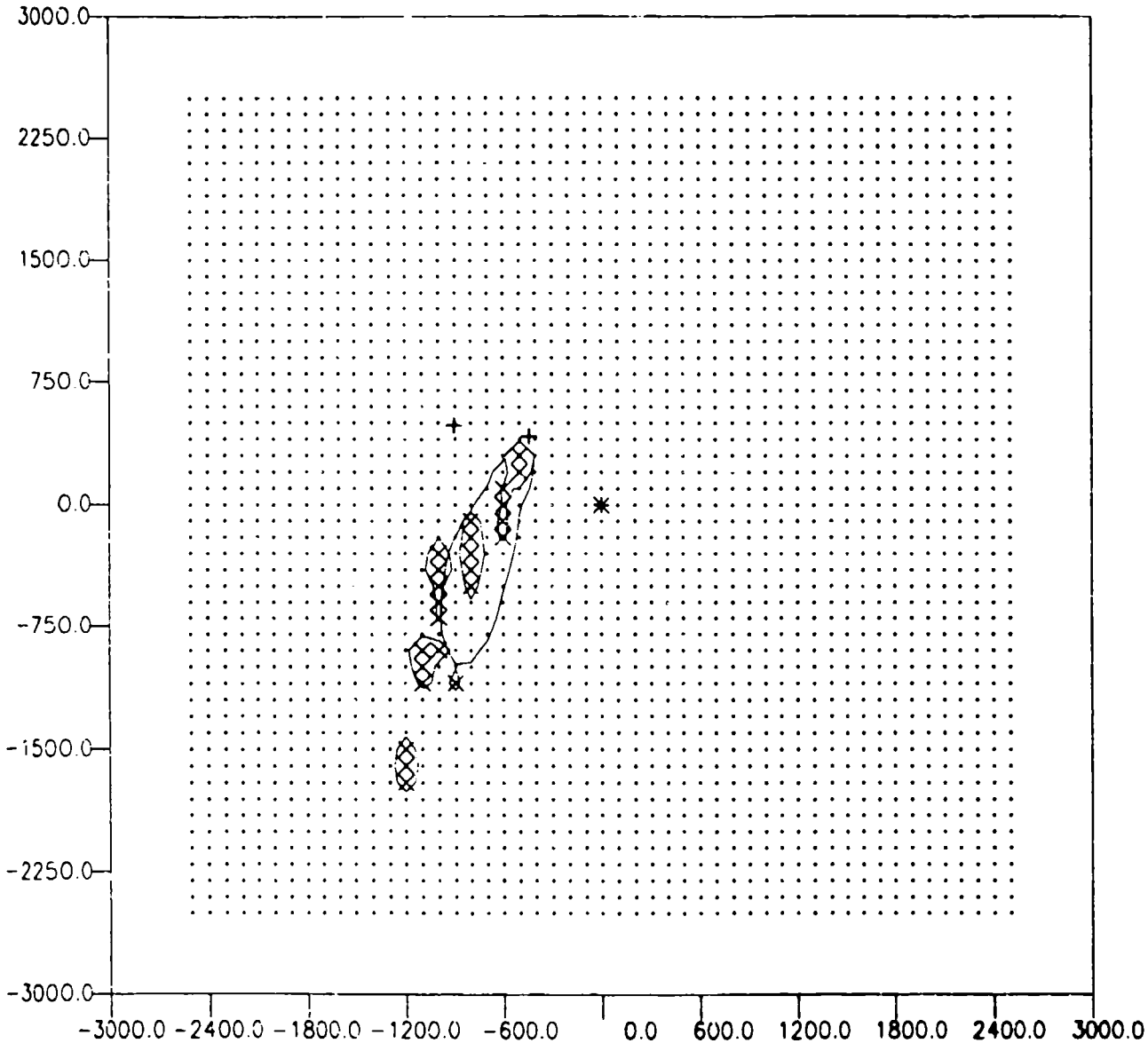

Figure A-24 Excursion 2 Trial A3, 40 mg/m^2

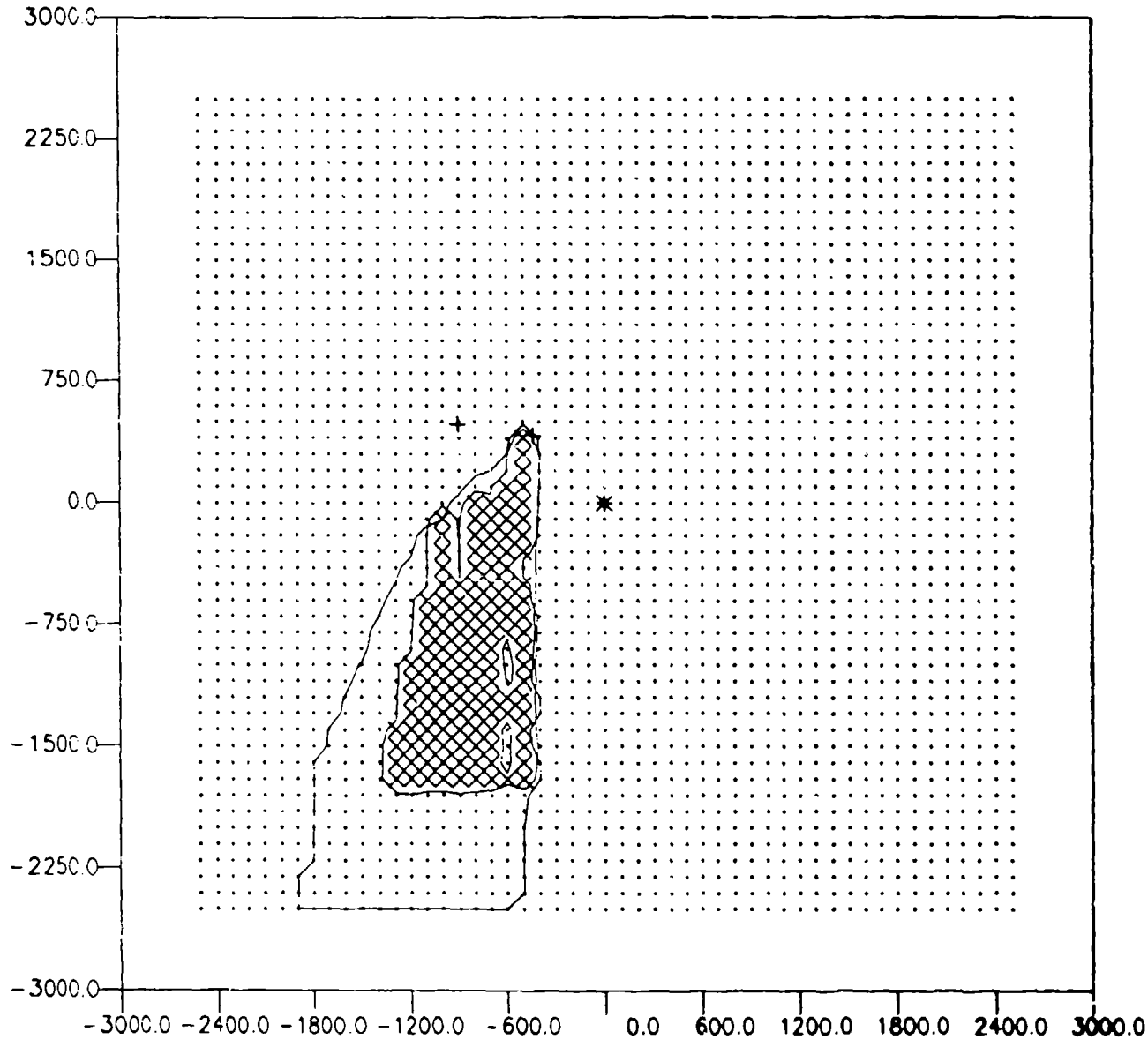

Figure A-25 Excursion 3 Trial A3, 1 mg/m^2

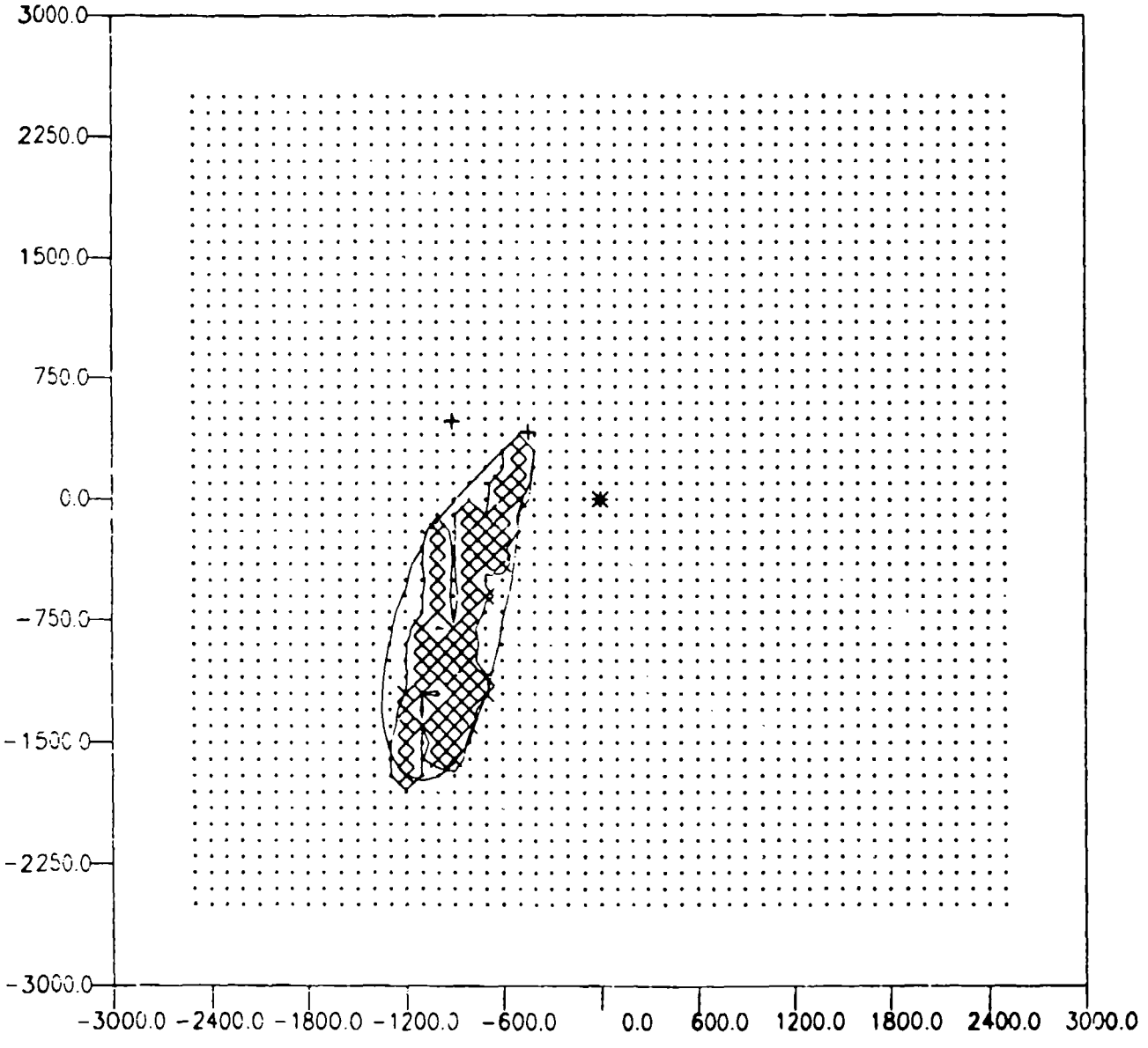

Figure A-26 Excursion 3 Trial A3, 10 mg/m^2

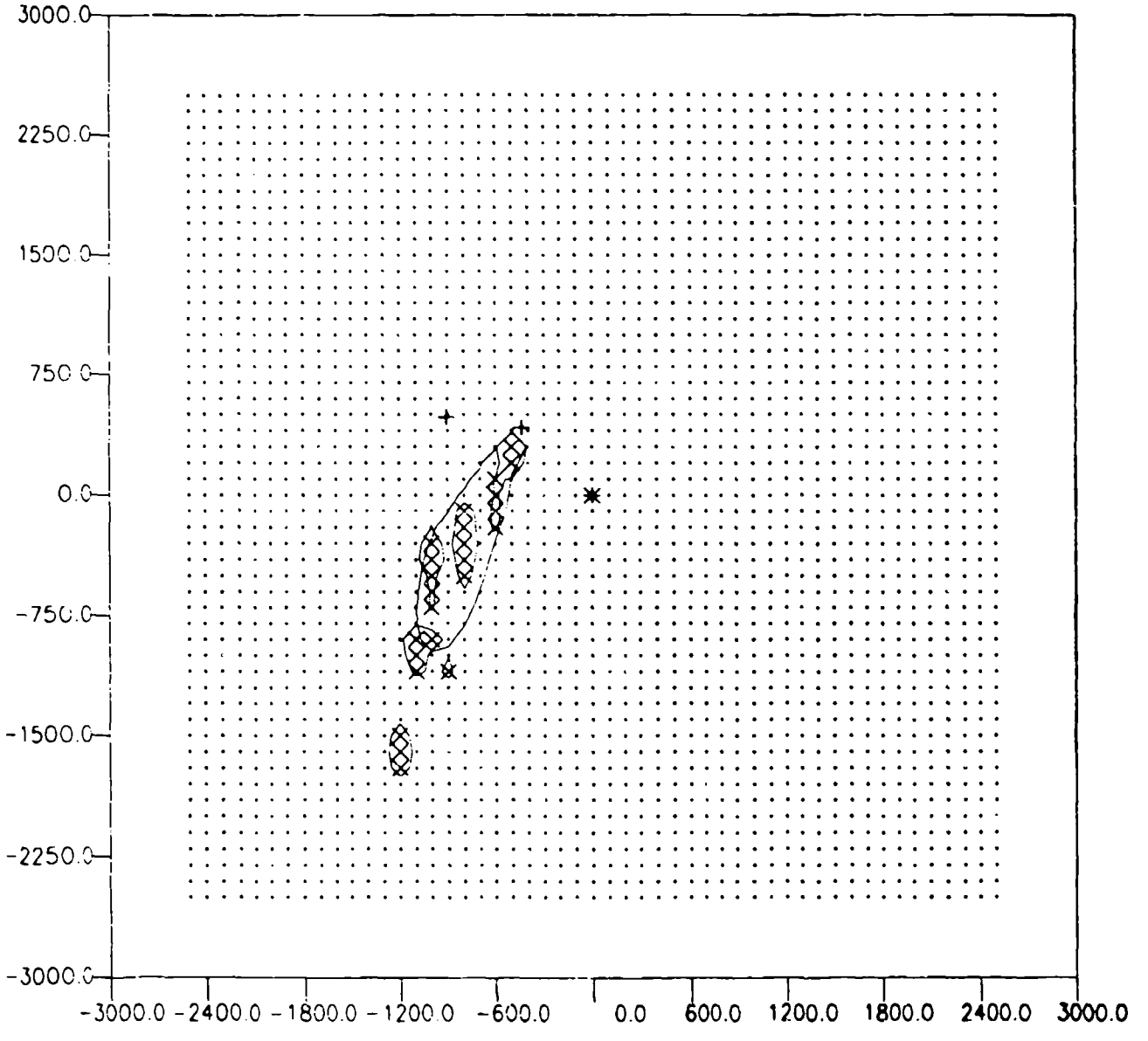

Figure A-27 Excursion 3 Trial A3, 40 mg/m^2

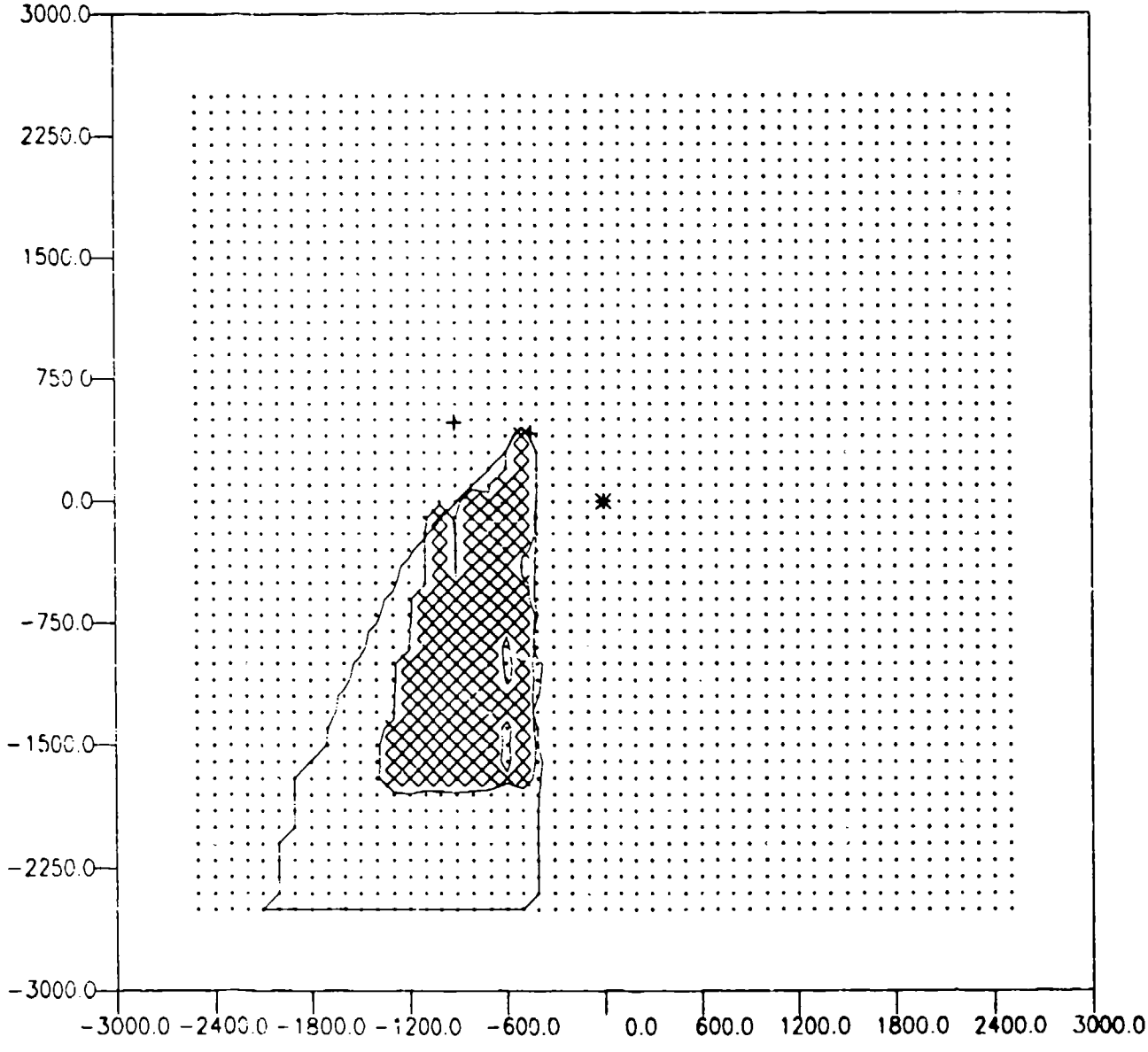

Figure A-28 Excursion 4 Trial A3, 1 mg/m^2

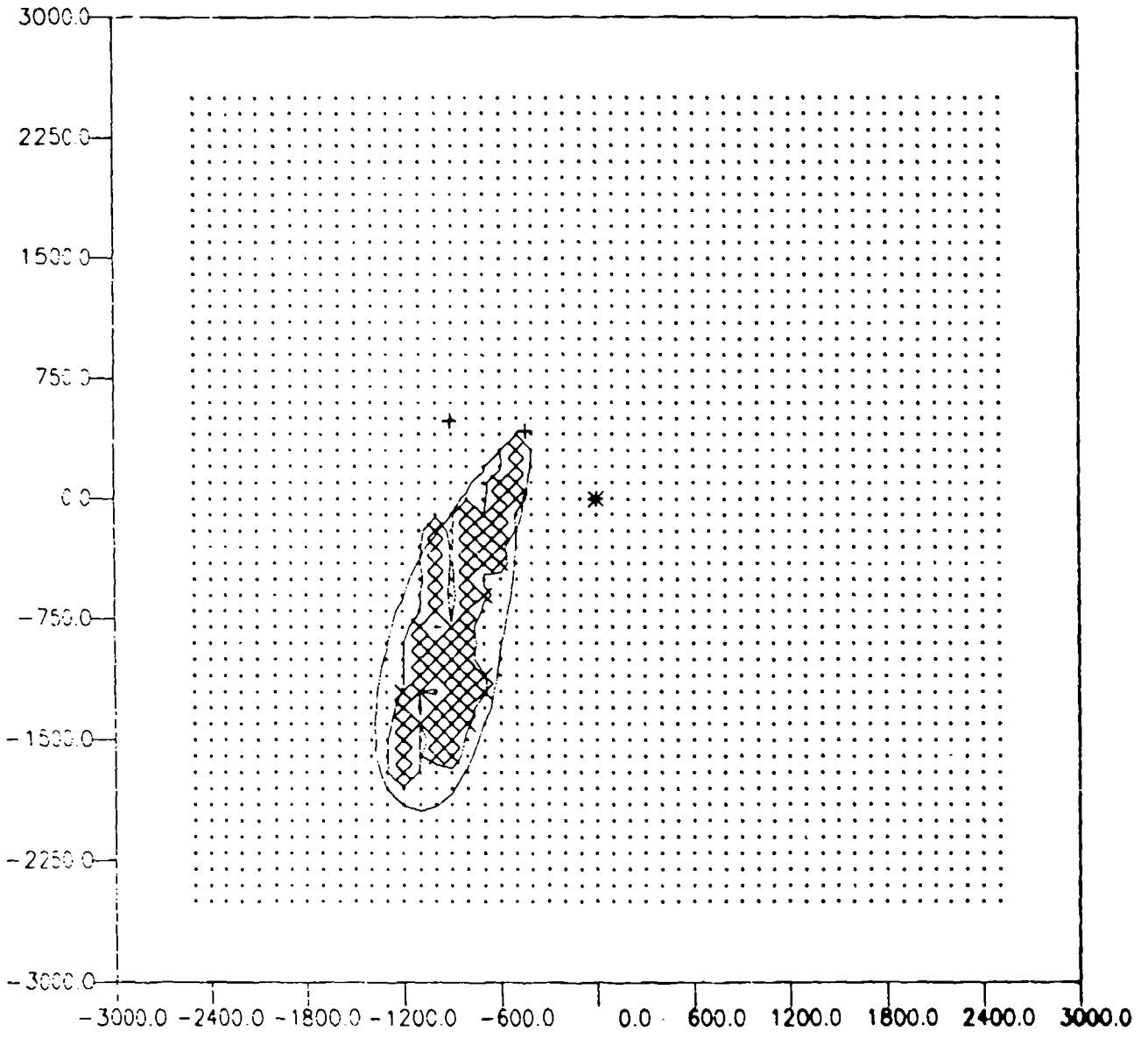

Figure A-29 Excursion 4 Trial A3, 10 mg/m^2

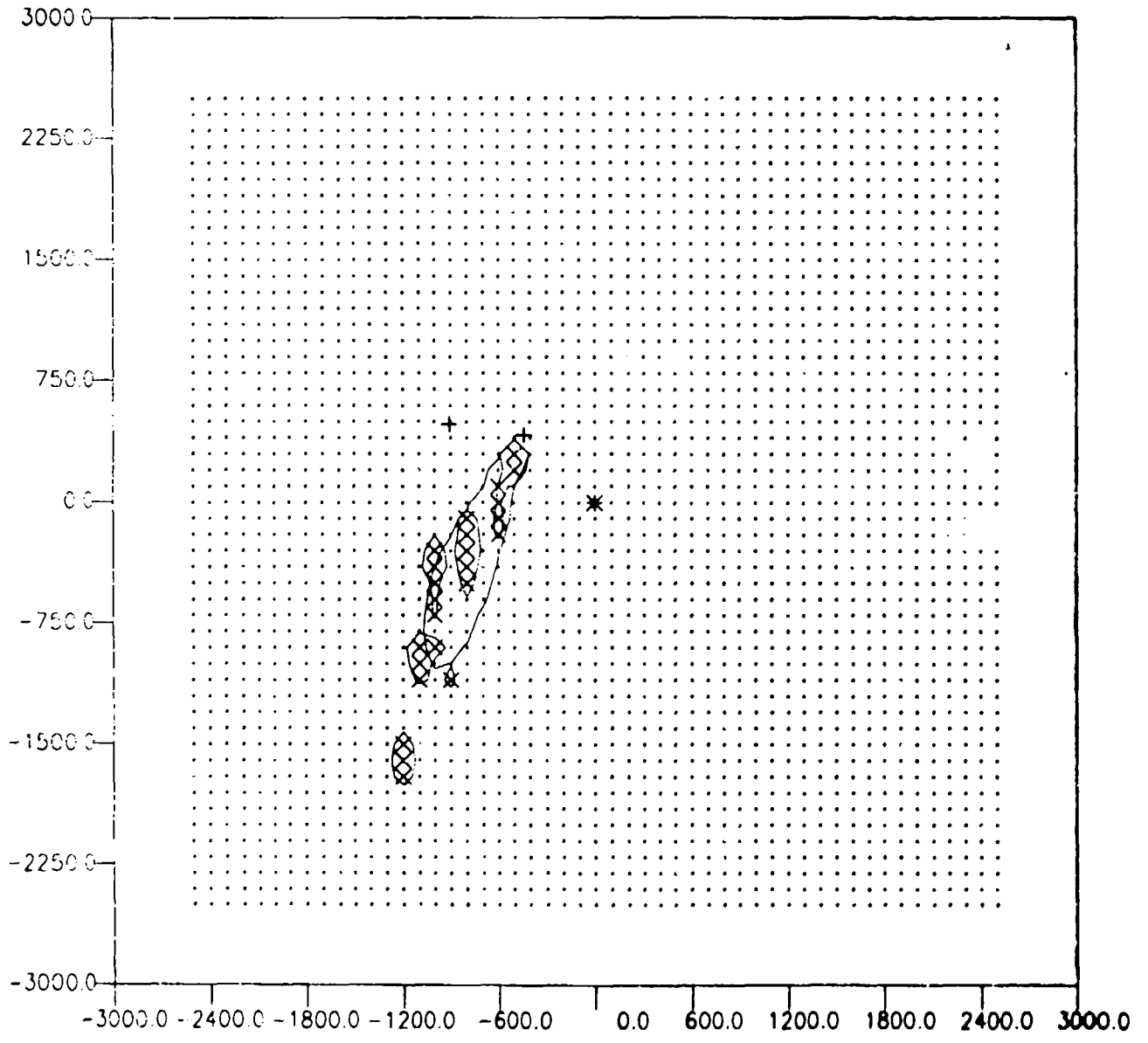

Figure A-30 Excursion 4 Trial A3, 40 mg/m^2

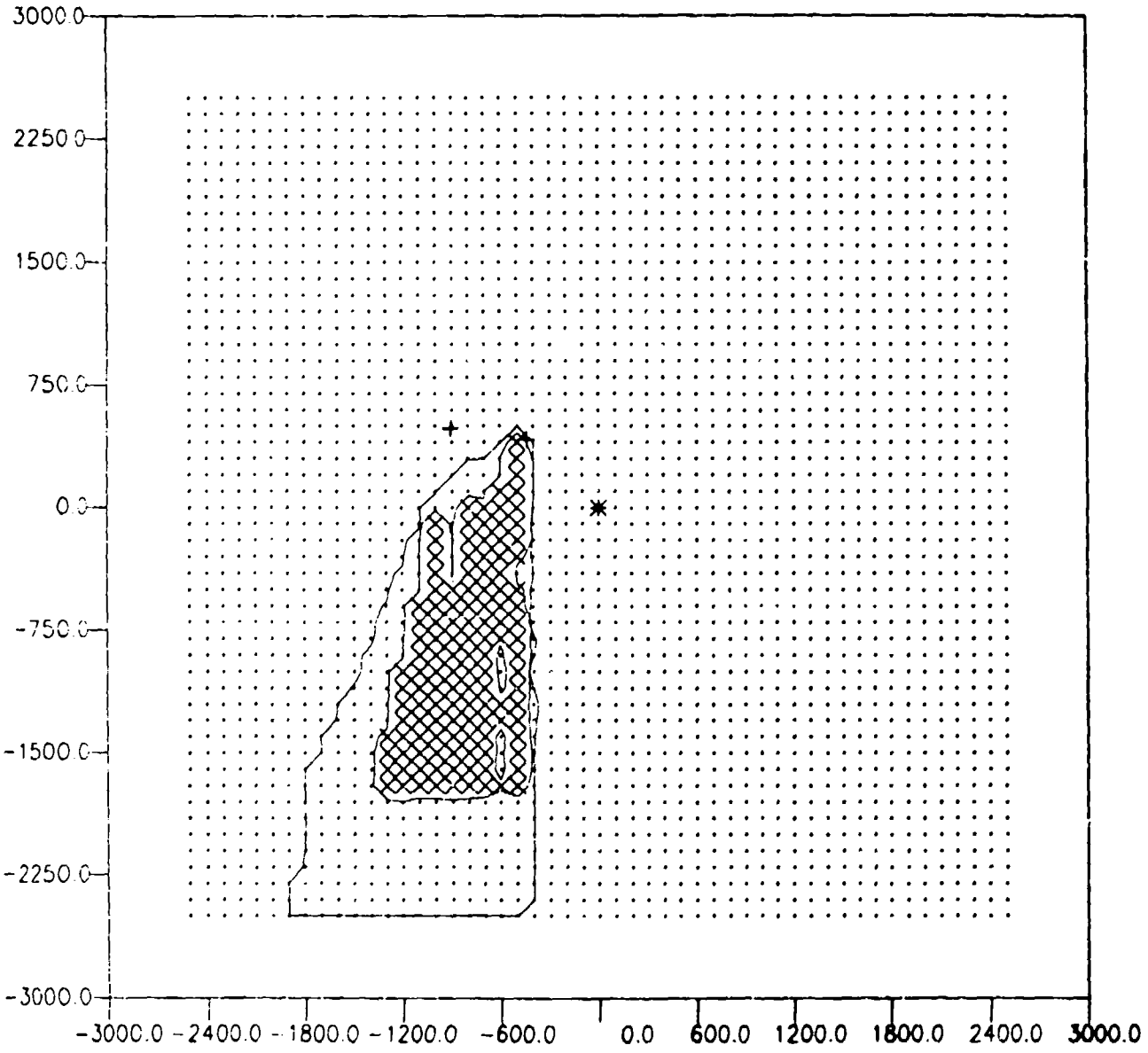

Figure A-31 Excursion 5 Trial A3, 1 mg/m^2

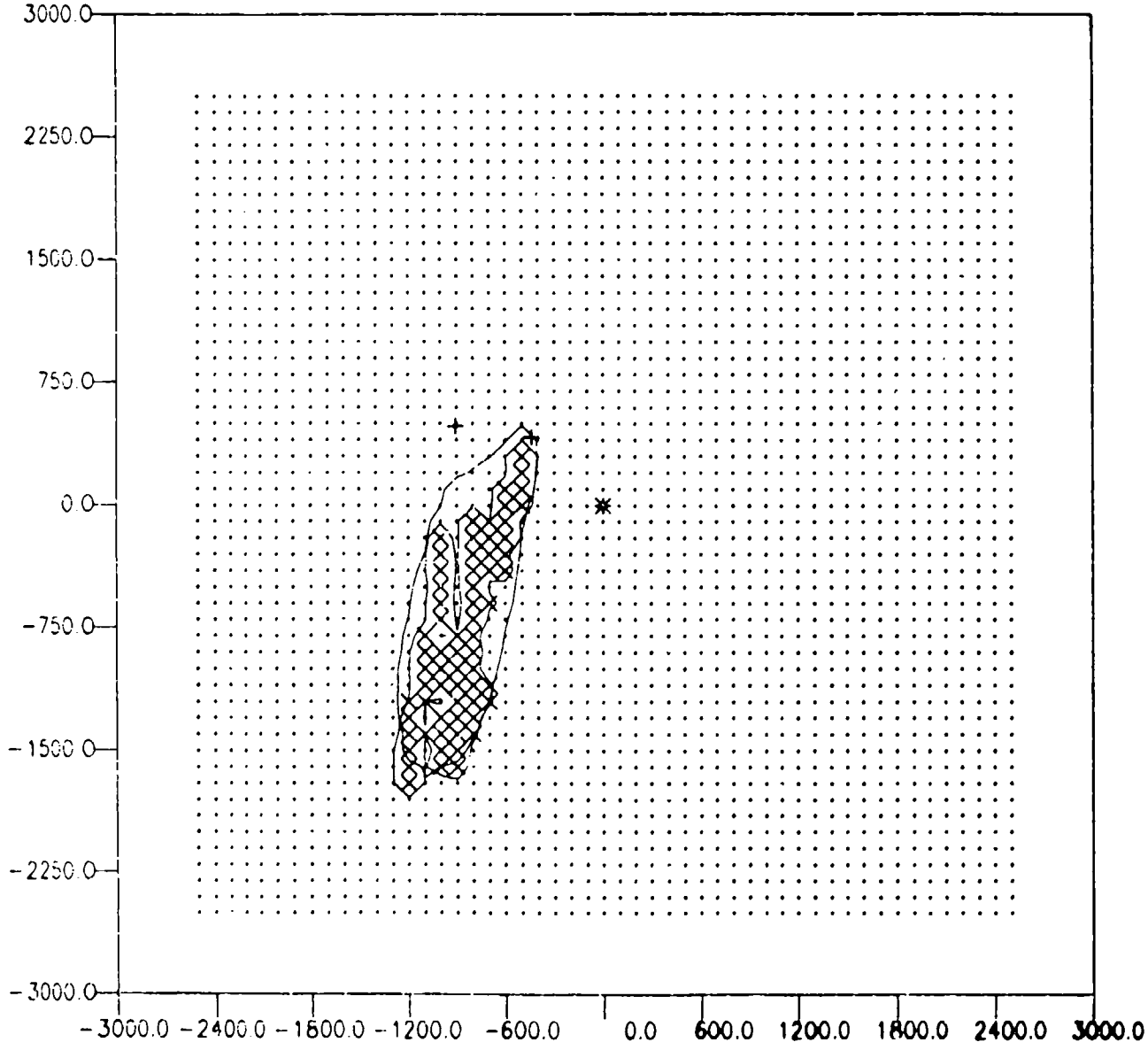

Figure A-32 Excursion 5 Trial A3, 10 mg/m^2

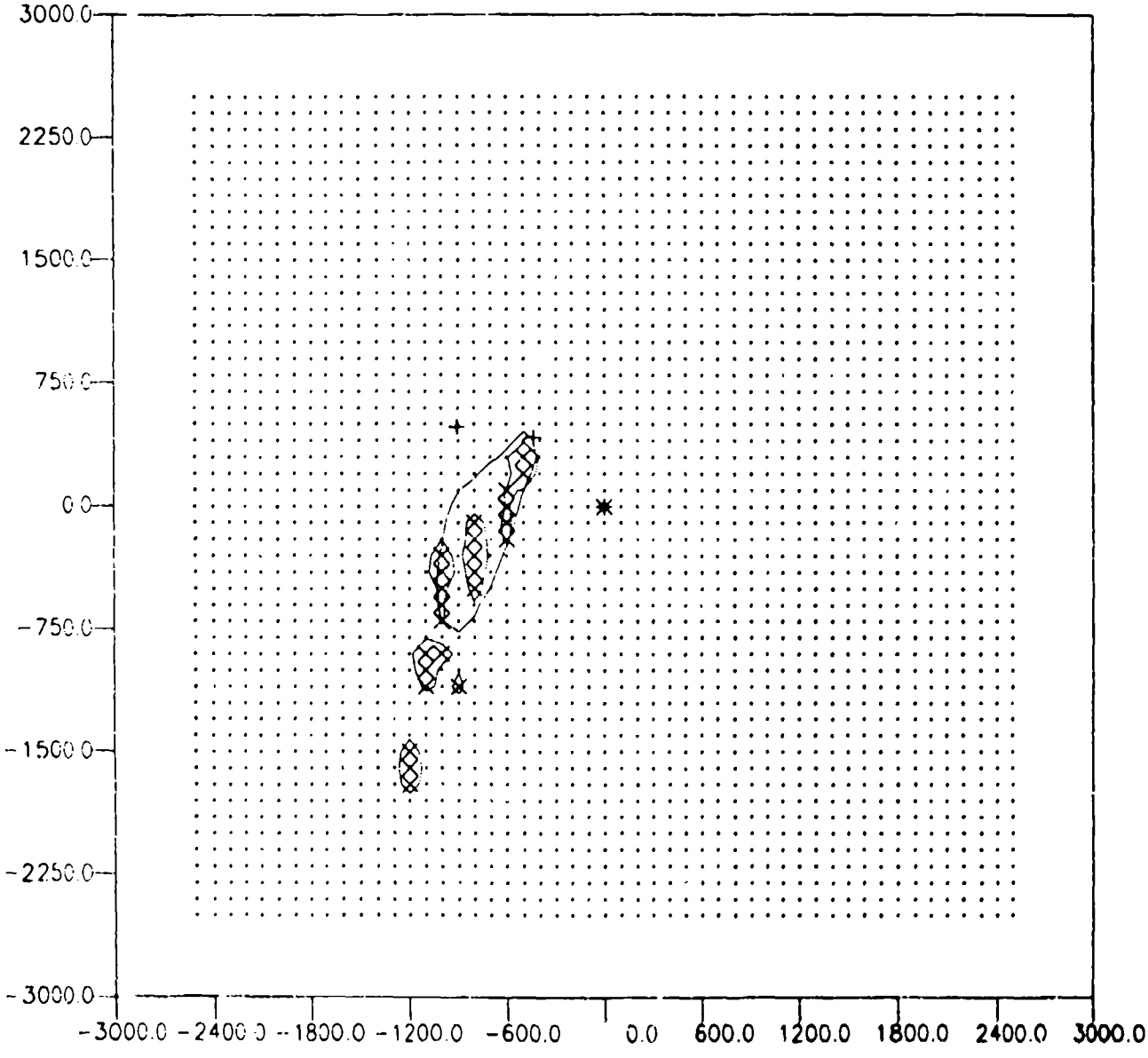

Figure A-33 Excursion 5 Trial A3, 40 mg/m^2

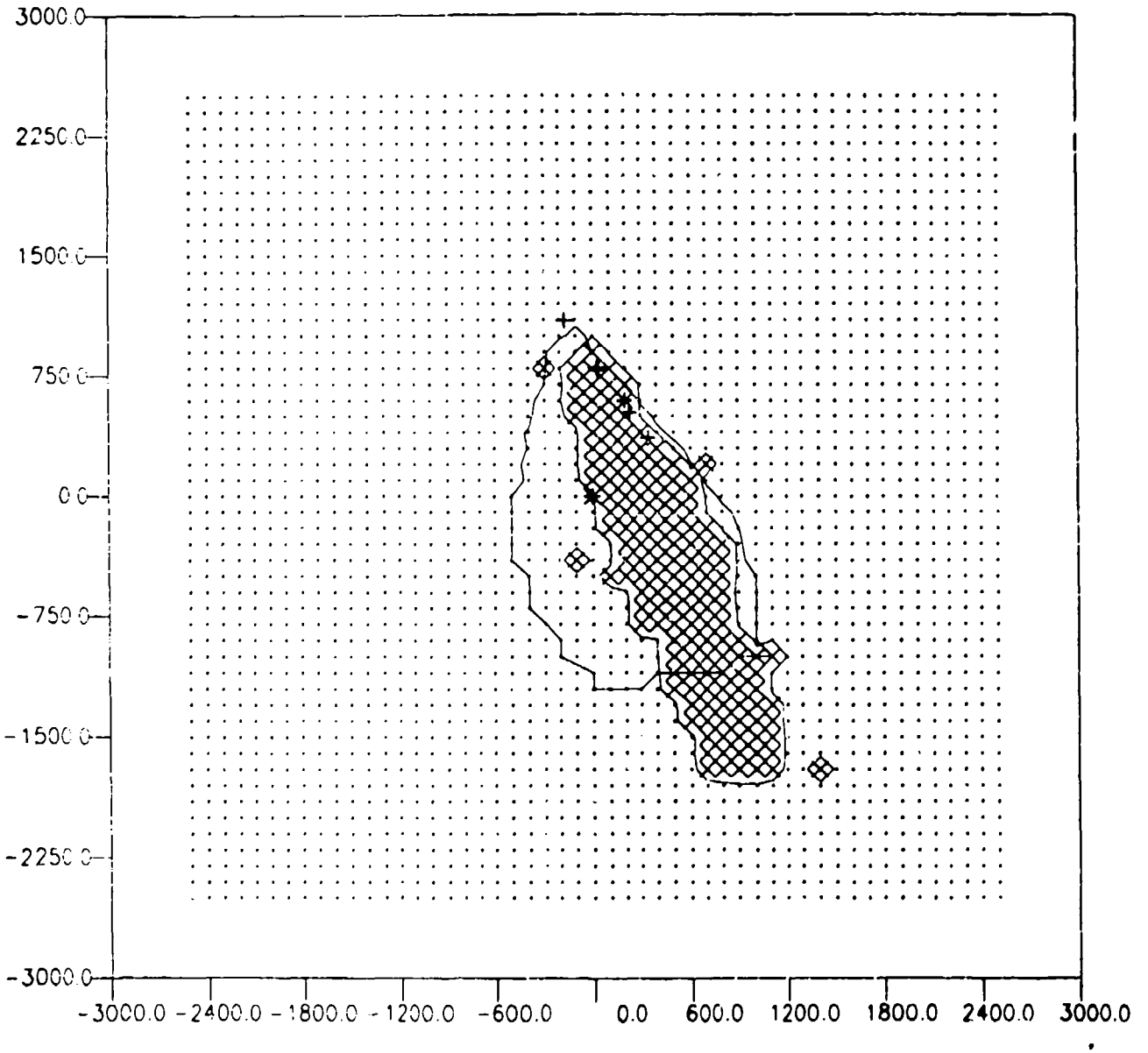

Figure A-34 Baseline Trial N8, 1 mg/m^2

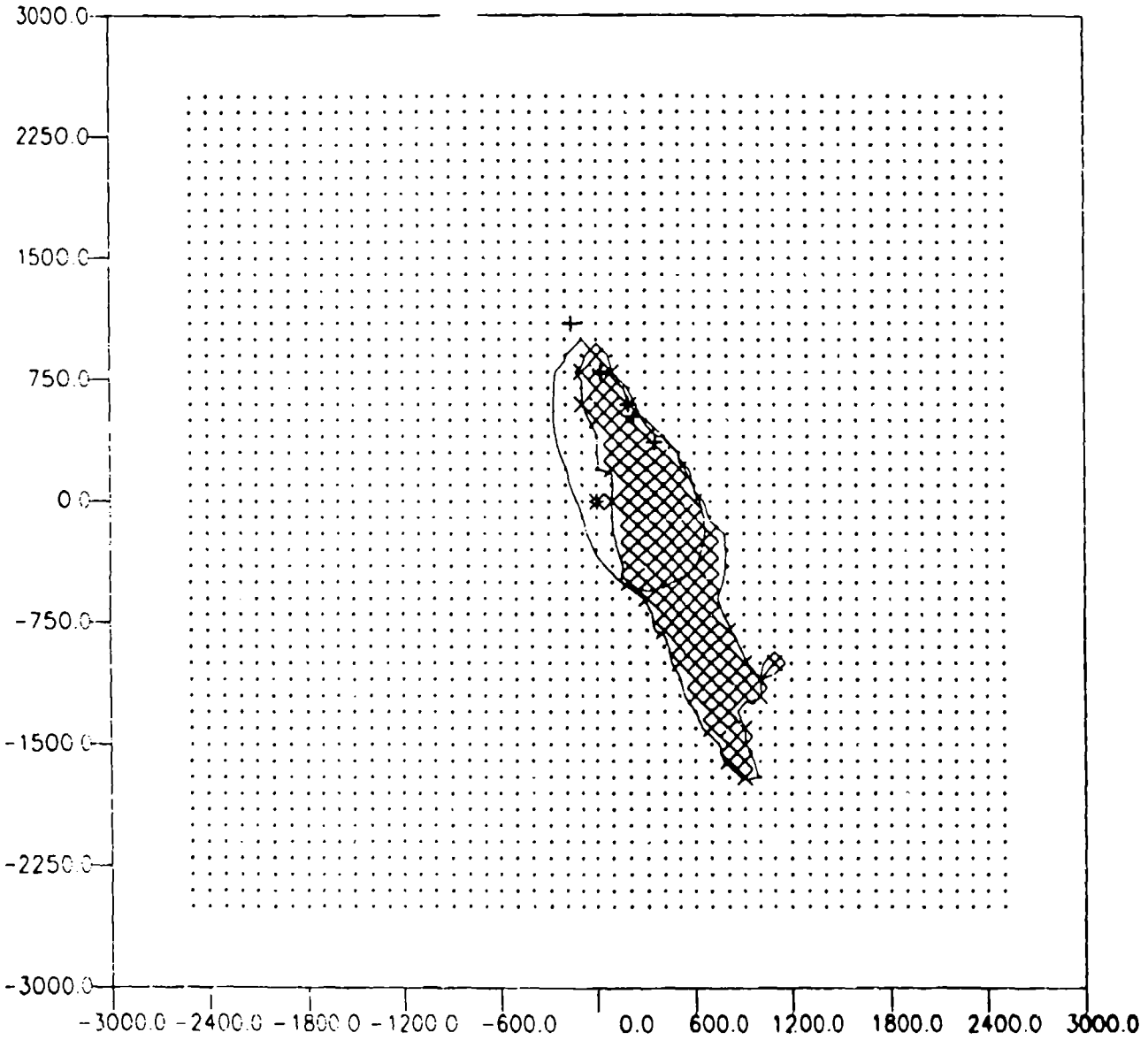

Figure A-35 Baseline Trial N8, 10mg/m^2

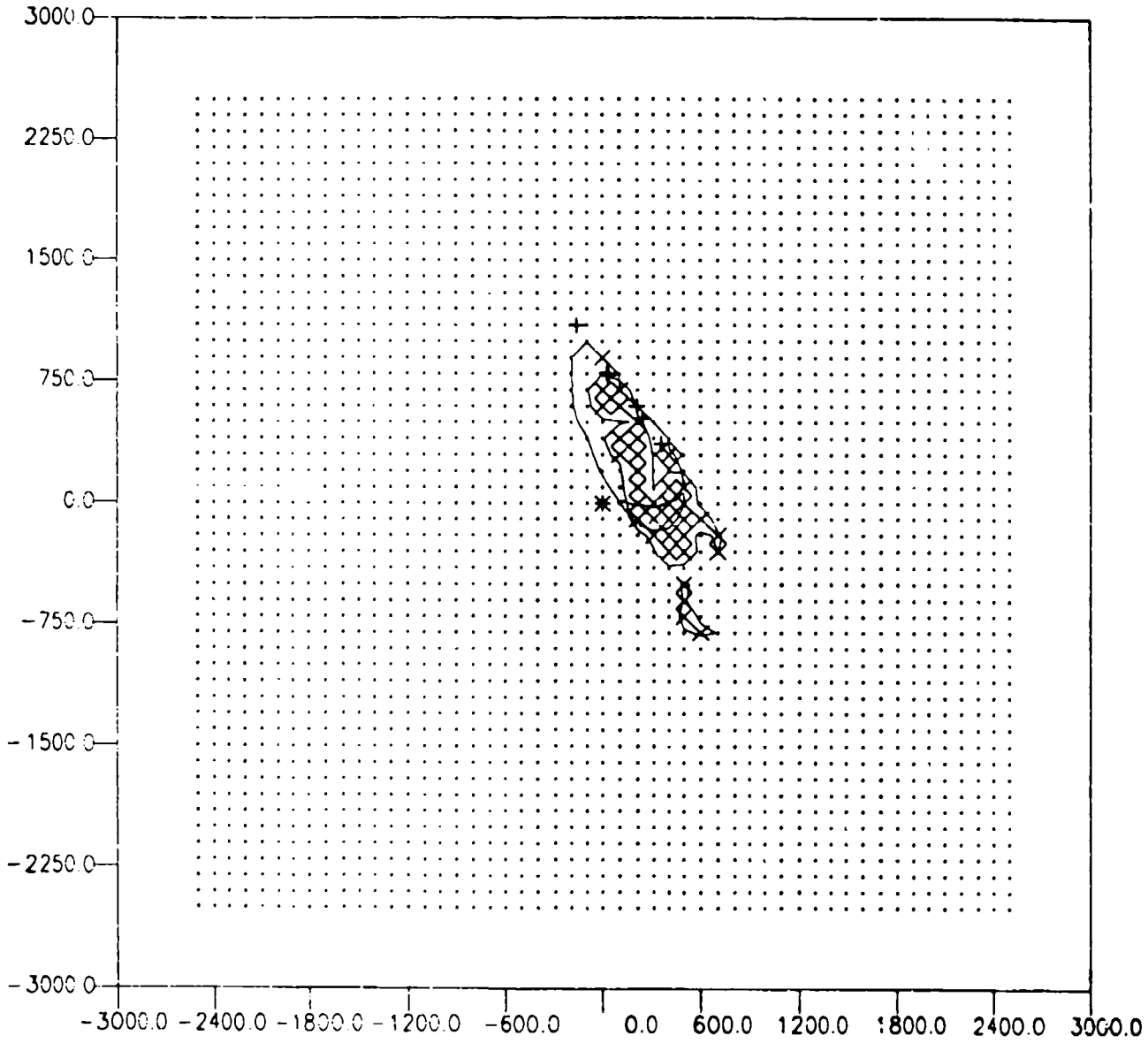

Figure A-36 Baseline Trial N8, 40mg/m^2

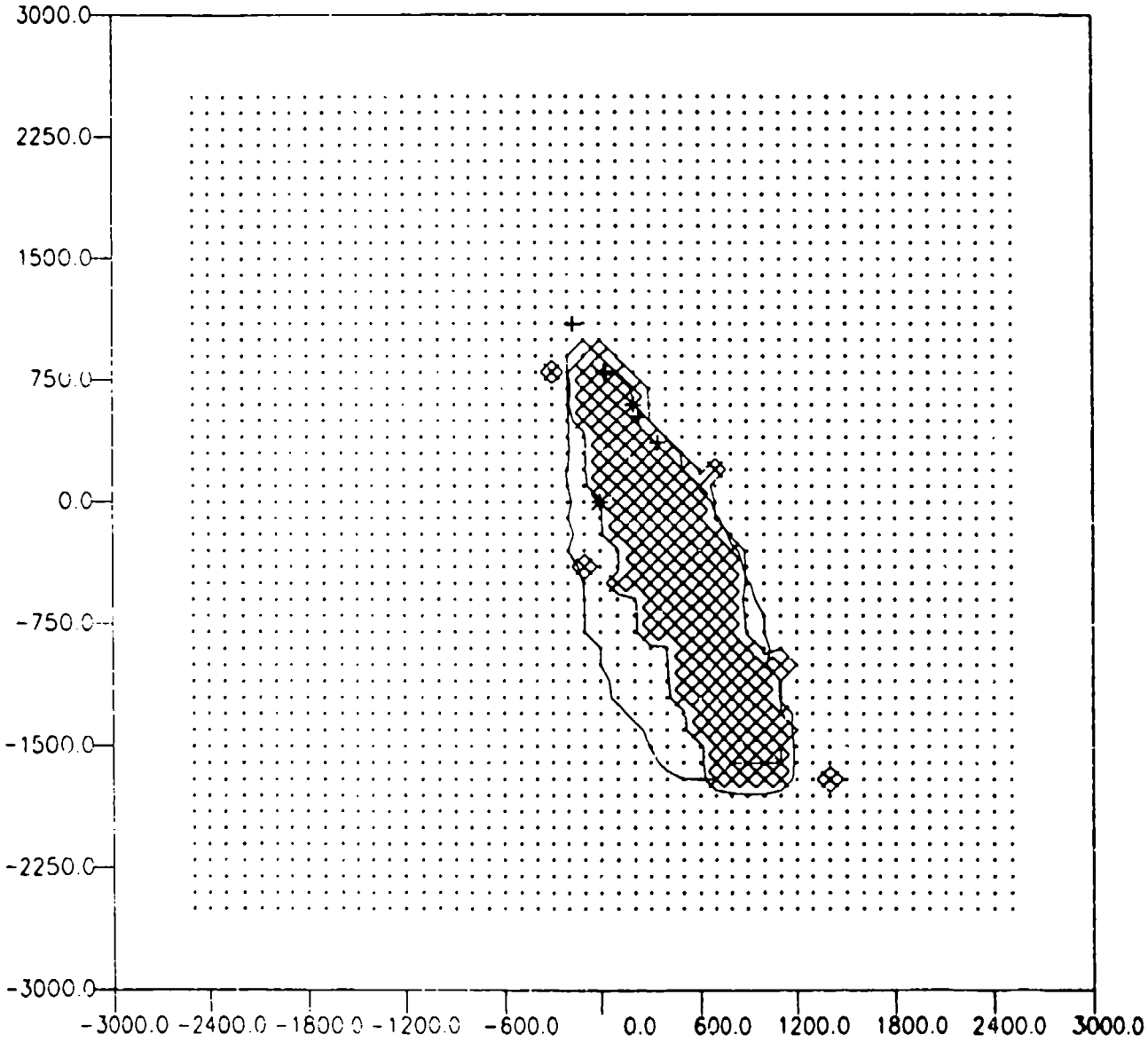

Figure A-37 Excursion Trial N8, 1 mg/m^2

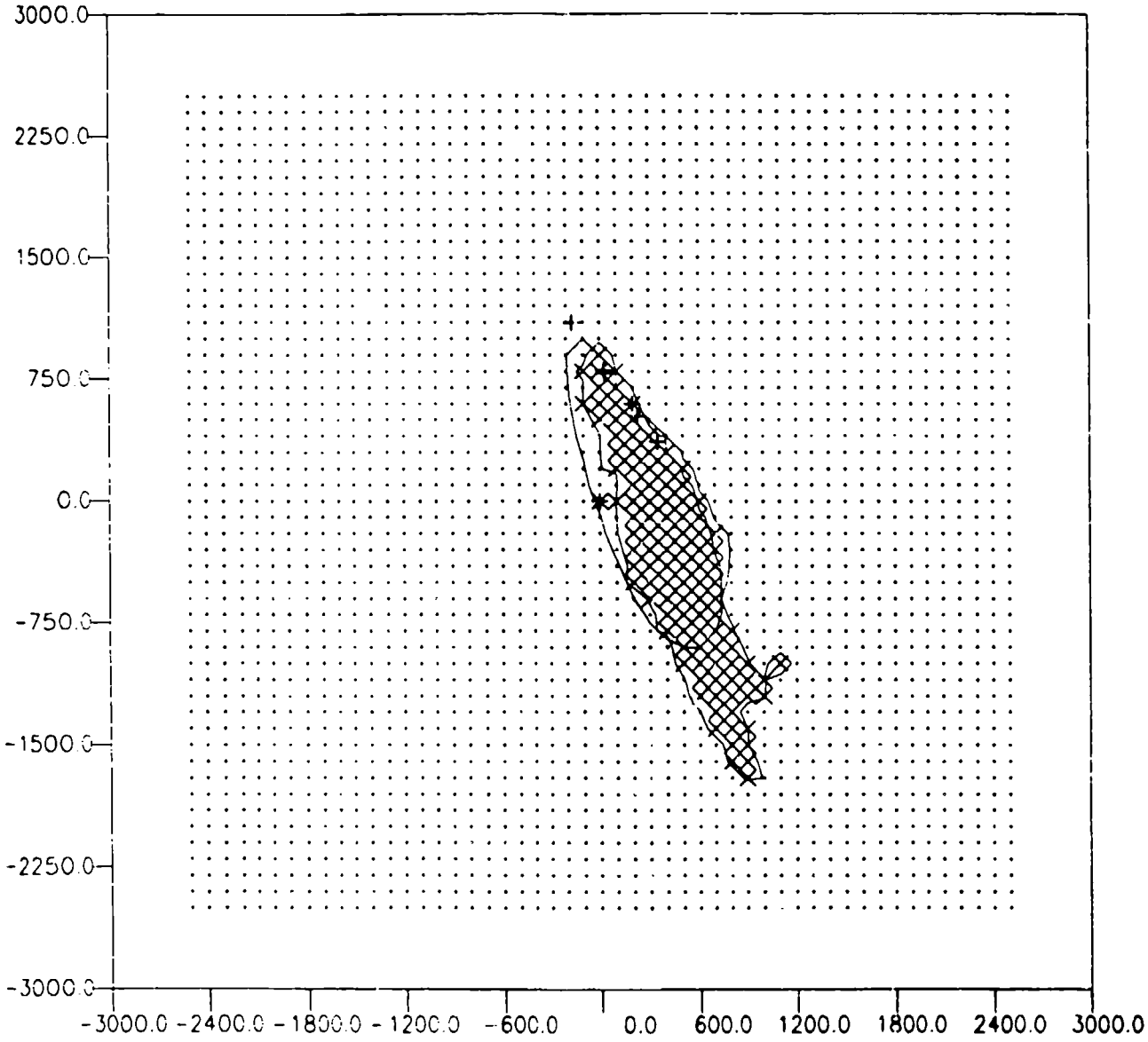

Figure A-38 Excursion Trial N8, 10 mg/m^2

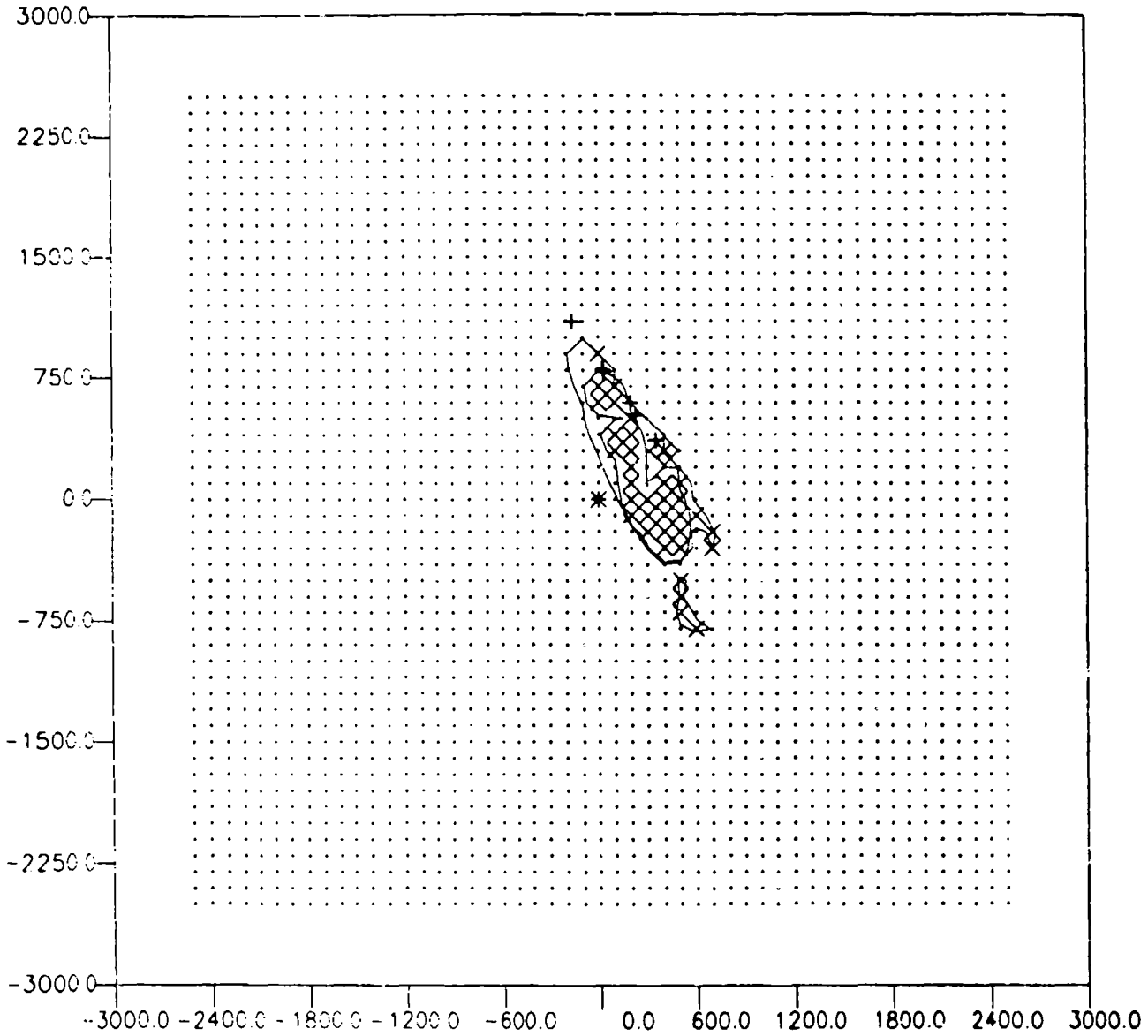

Figure A-39 Excursion Trial N8, 40 mg/m^2

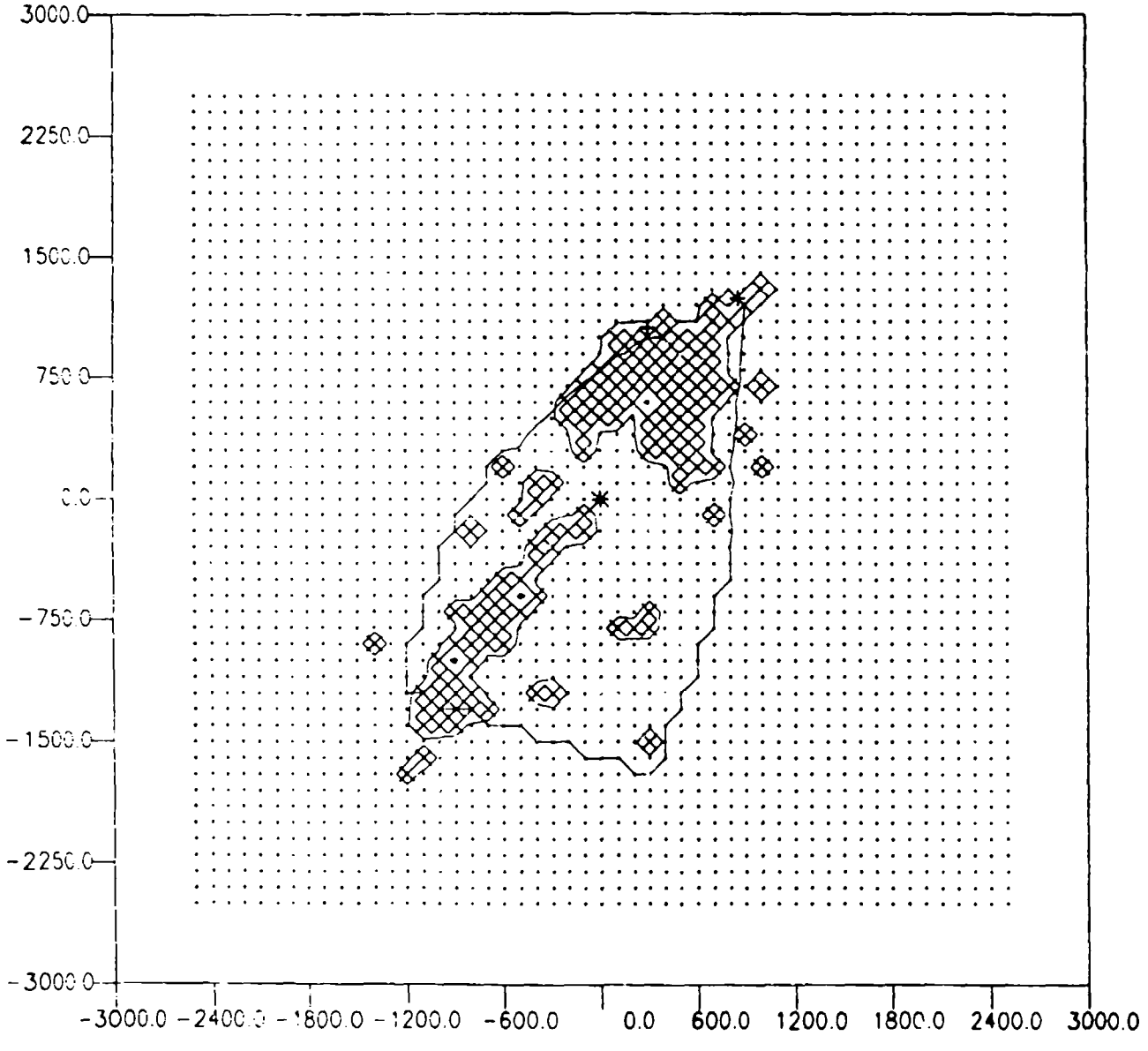

Figure A-40 Baseline Trial N3, 1mg/m^2

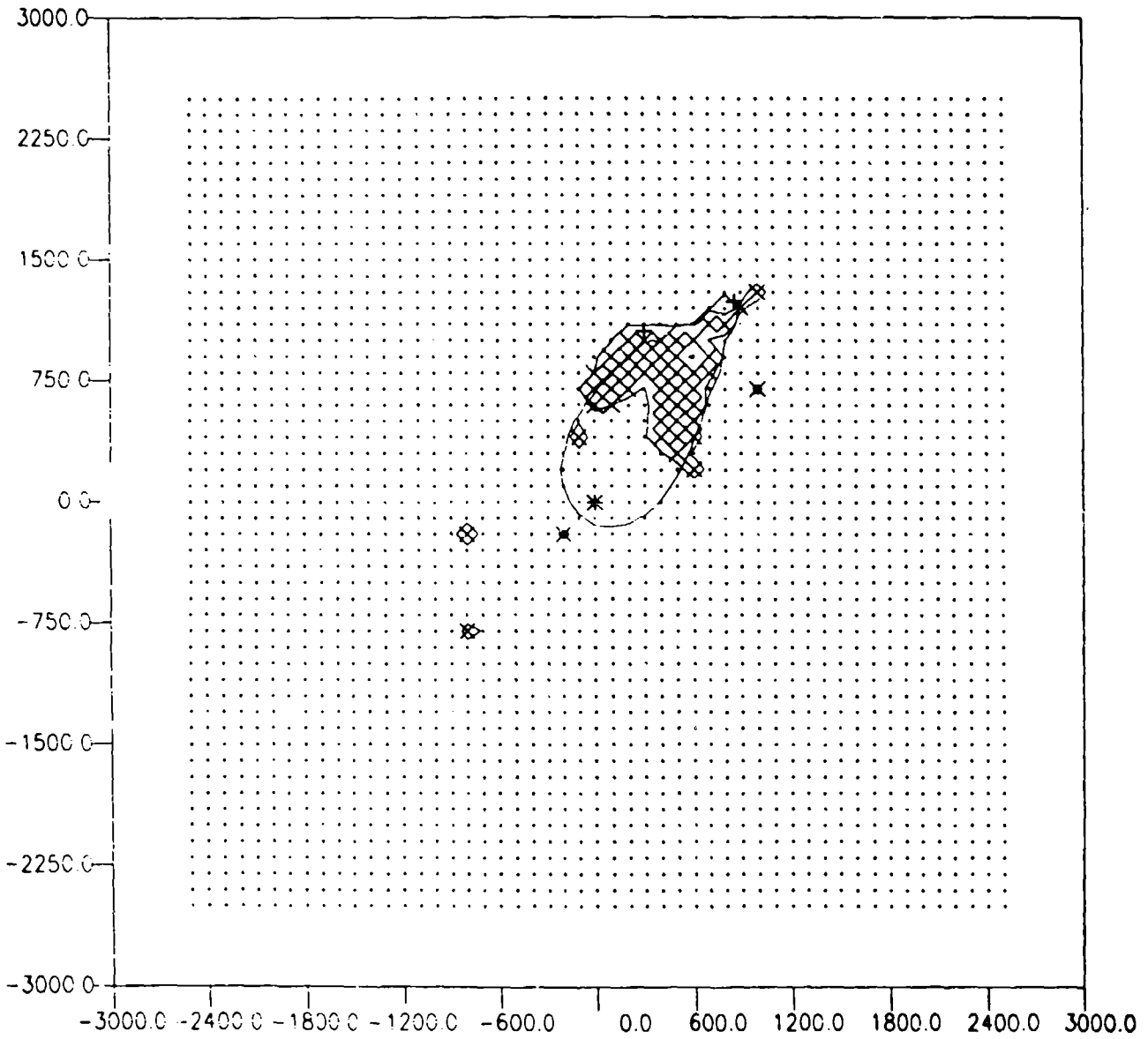

Figure A-41 Baseline Trial N3, 10 mg/m^2

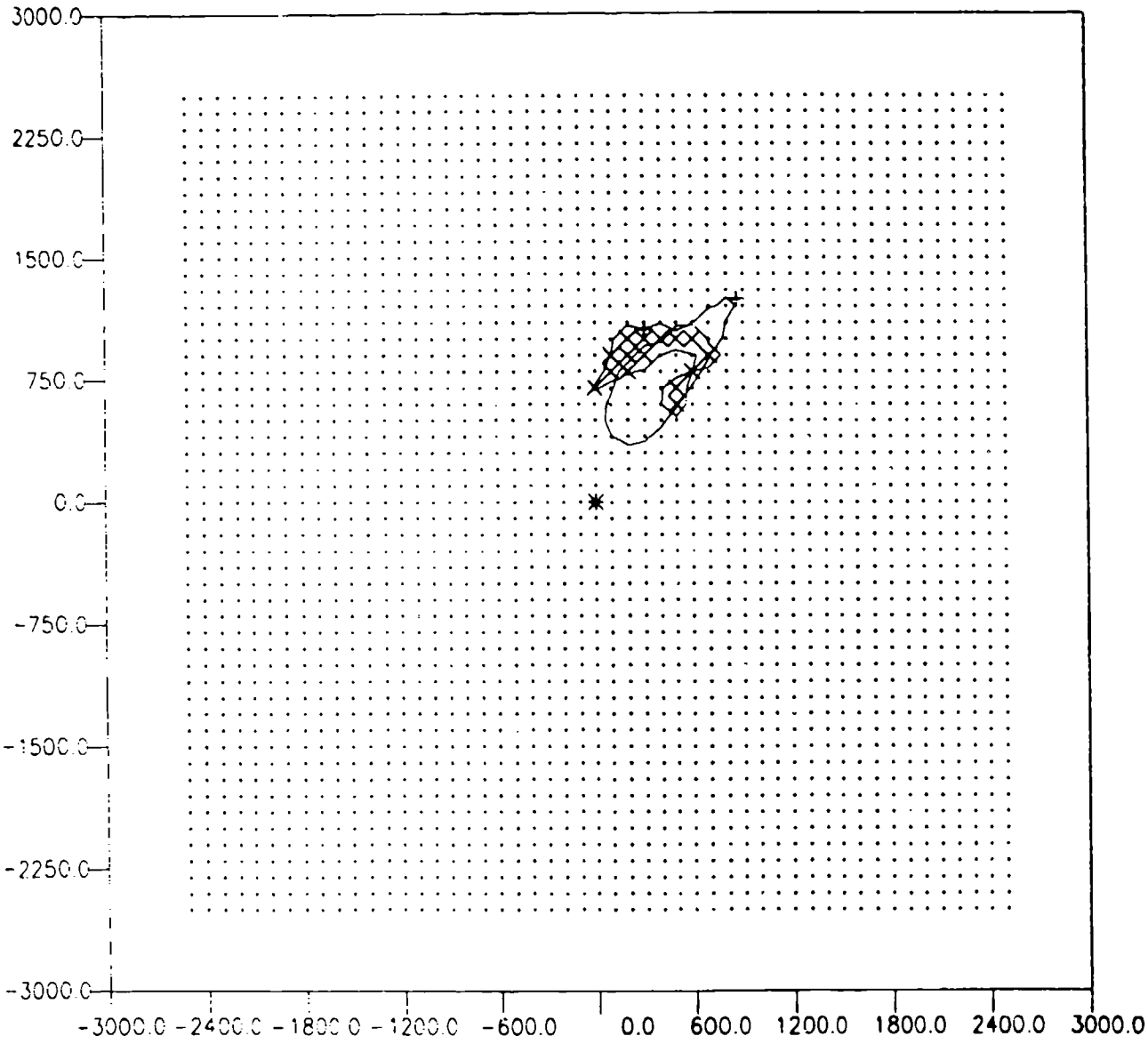

Figure A-42 Baseline Trial N3, 40 mg/m^2

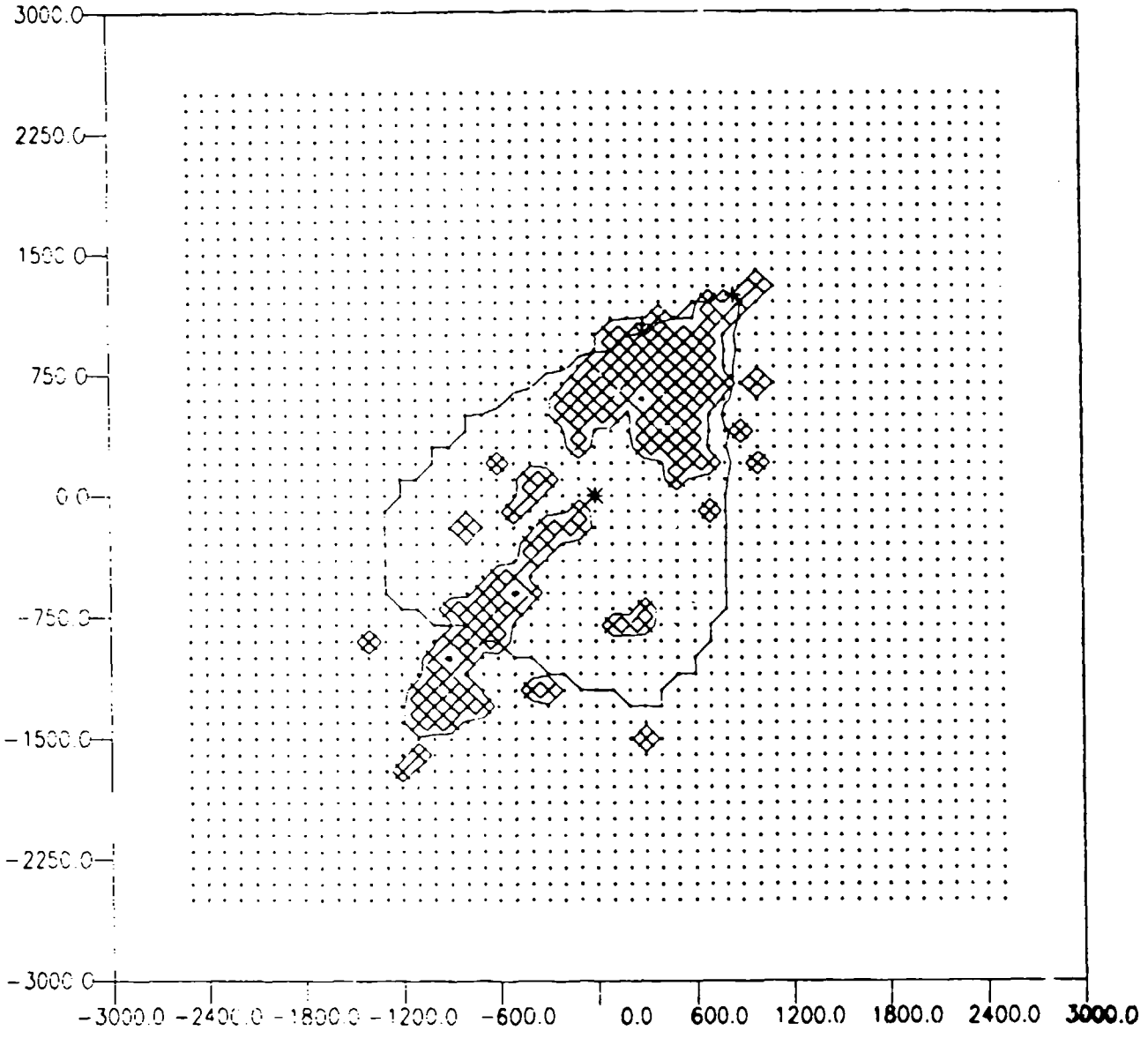

Figure A-43 Excursion Trial N3, 1 mg/m^2

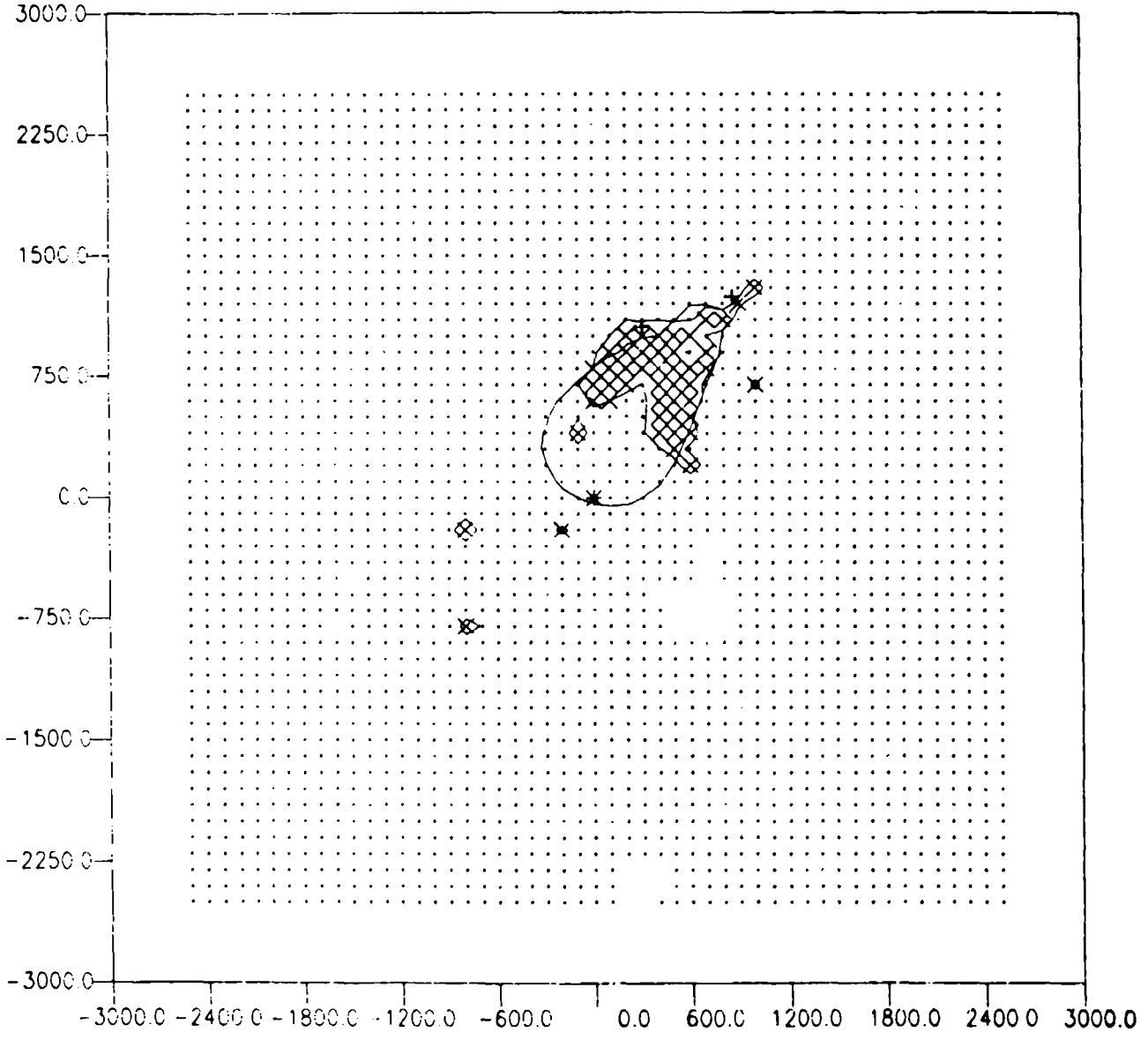

Figure A-44 Excursion Trial N3, 10 mg/m^2

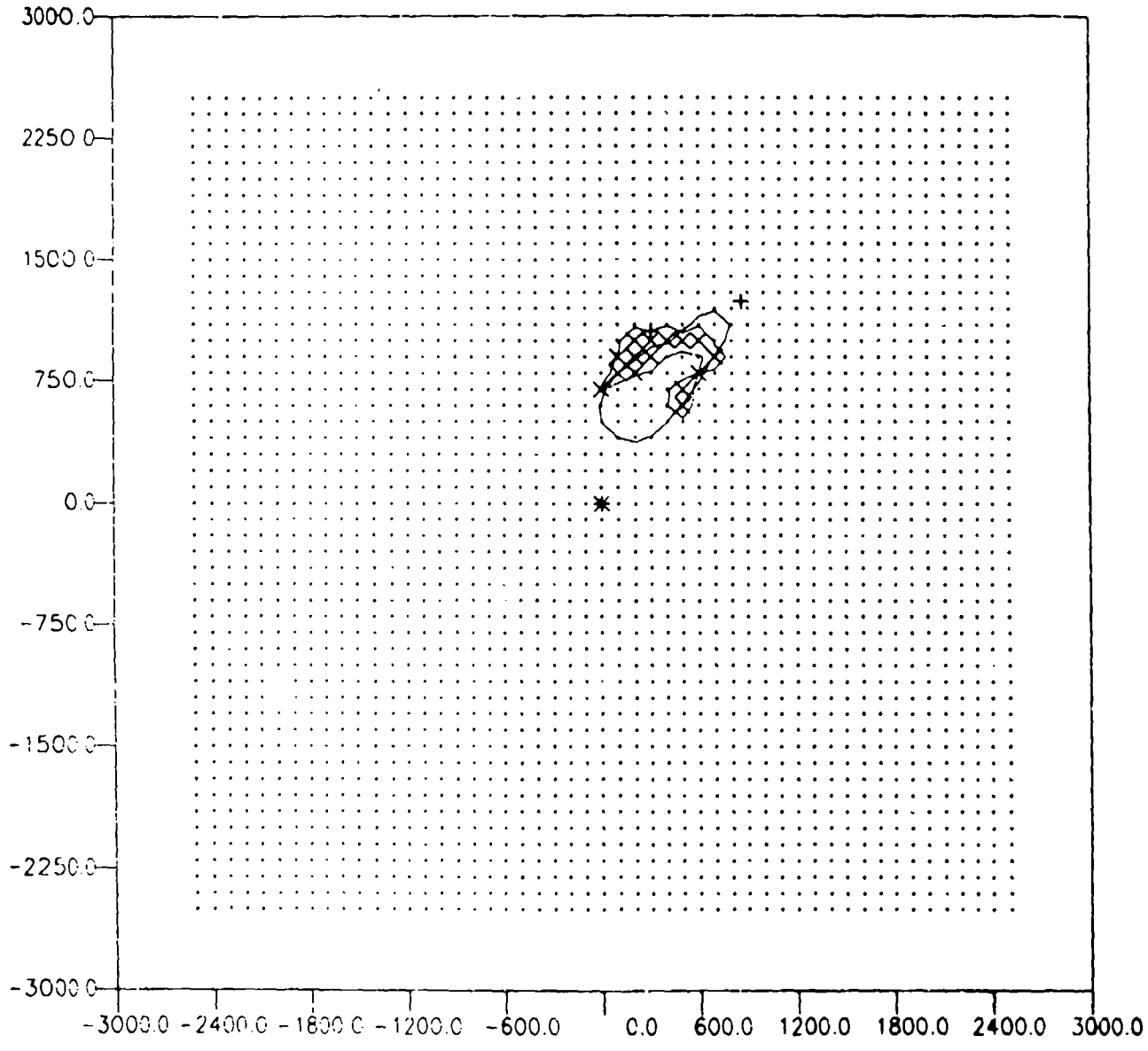

Figure A-45 Excursion Trial N3, 40 mg/m^2

APPENDIX B

A/D Plots

Each plot depicts the experimental and predicted data for the baseline and excursion of each trial.

Figures B-1 - B-2	Trial N4
Figures B-3 - B-4	Trial A1
Figures B-5 - B-6	Trial N6
Figures B-7 - B-12	Trial A3
Figures B-13 - B-14	Trial N8
Figures B-15 - B-16	Trial N3

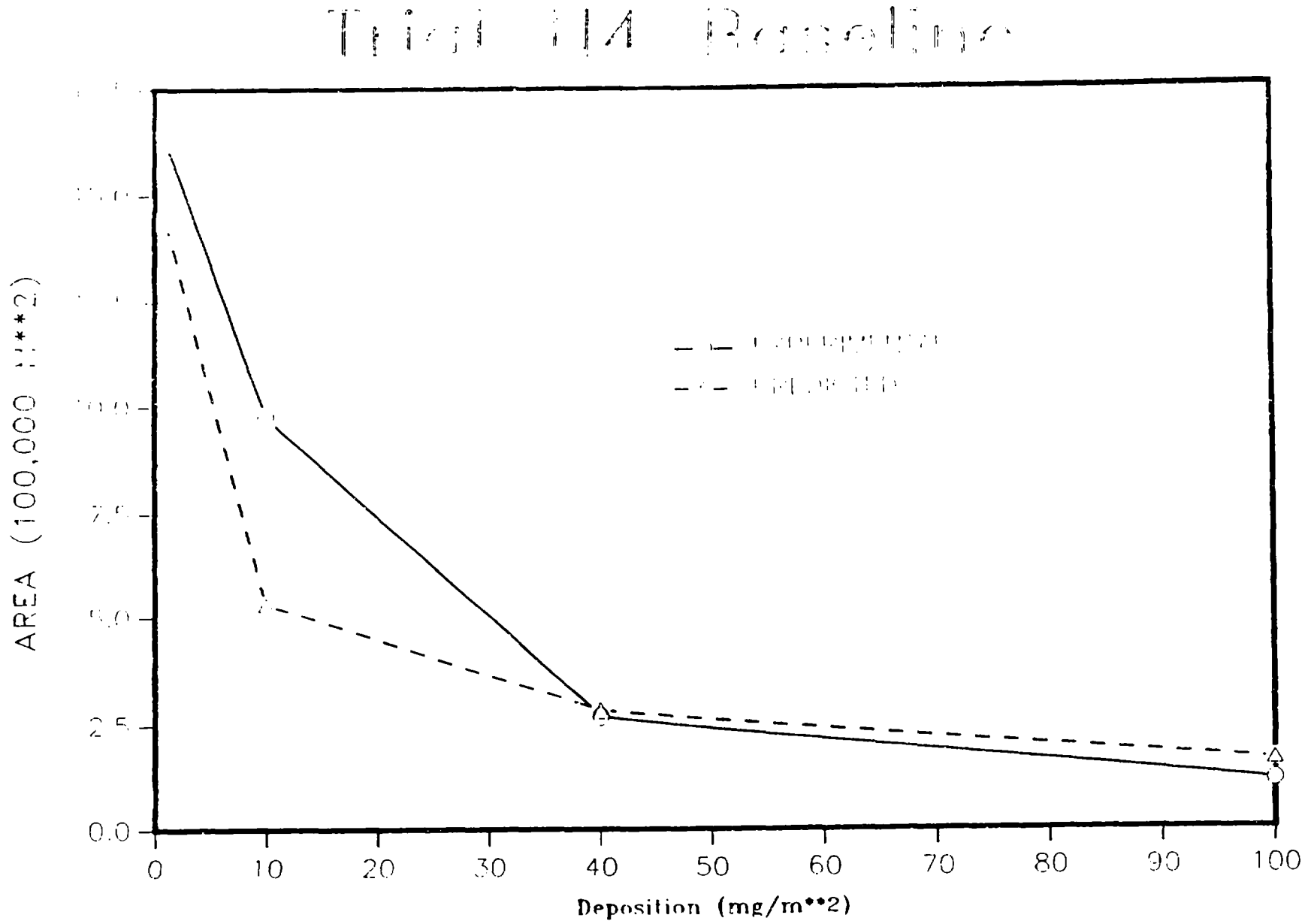
AREA (100,000 ft**2)
0.0
2.5
5.0
0
10
20
30
40
50
60
70
80
90
100
Deposition (mg/m**2)

Figure B-1

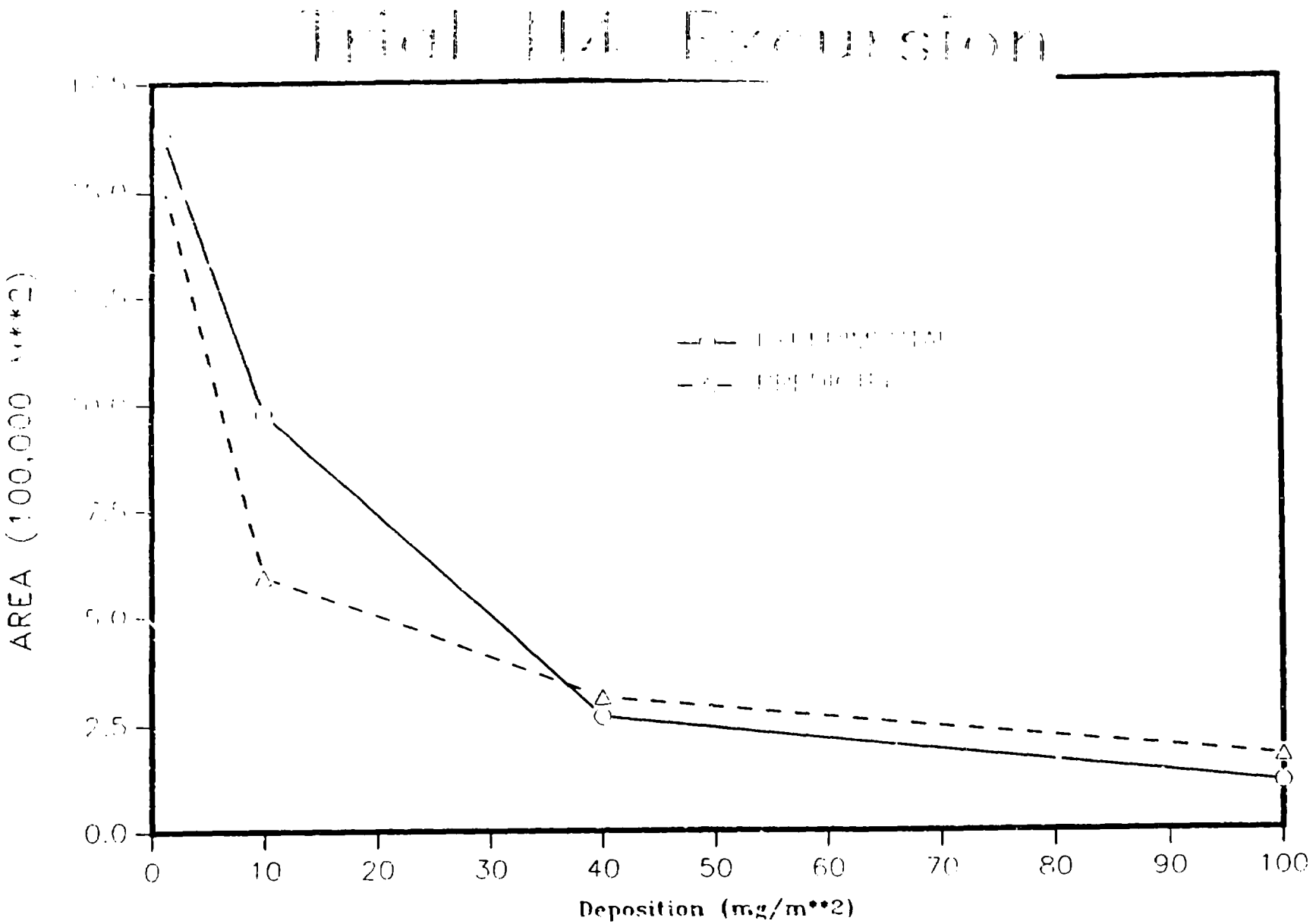
AREA (100,000 ft**2)
0.0
2.5
5.0
0
10
20
30
40
50
60
70
80
90
100
Deposition (mg/m**2)

Figure B-2

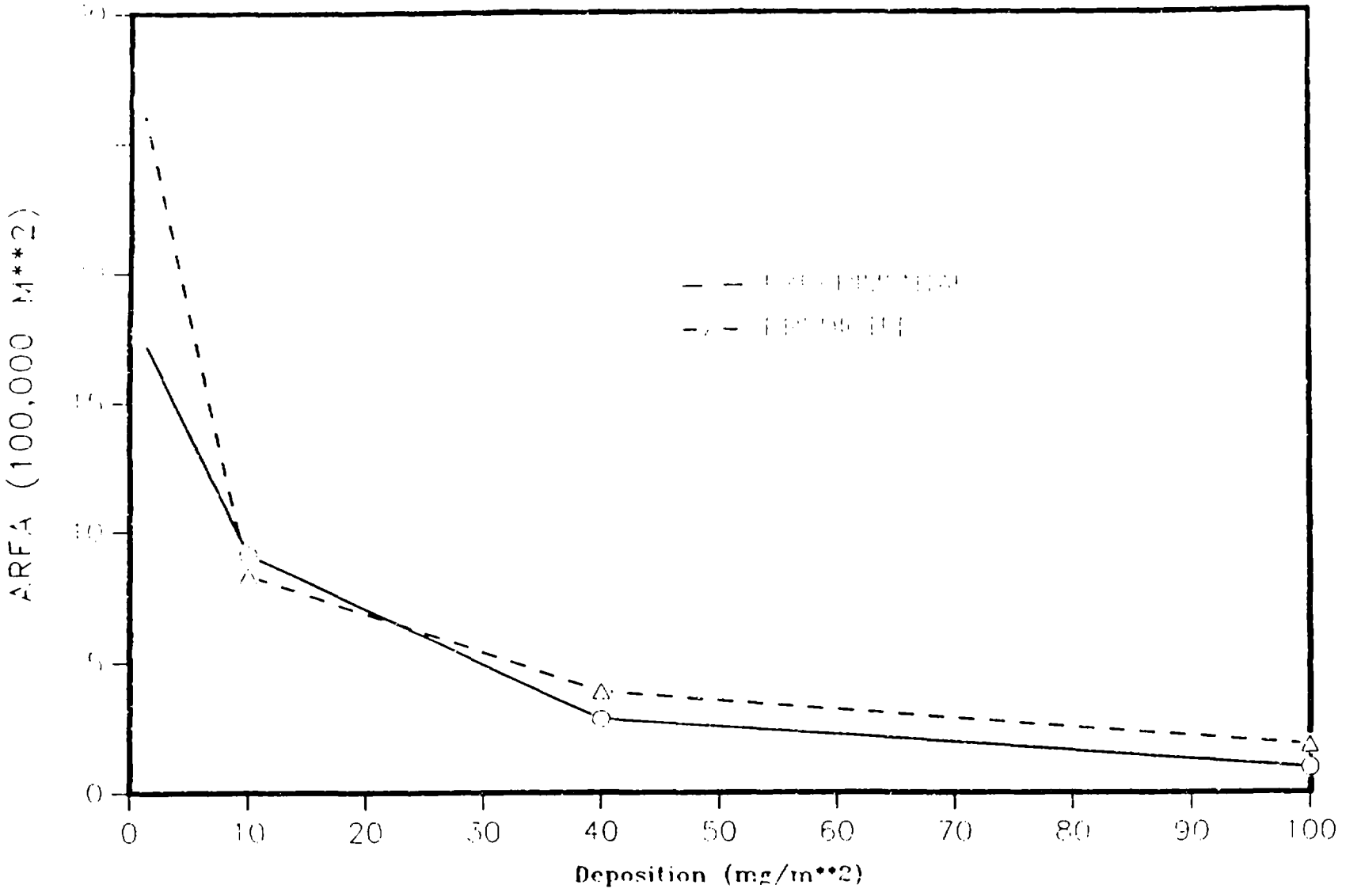
AREA (100,000 M**2)
0
5
10
15
0
10
20
30
40
50
60
70
80
90
100
Deposition (mg/m**2)

Figure B-3

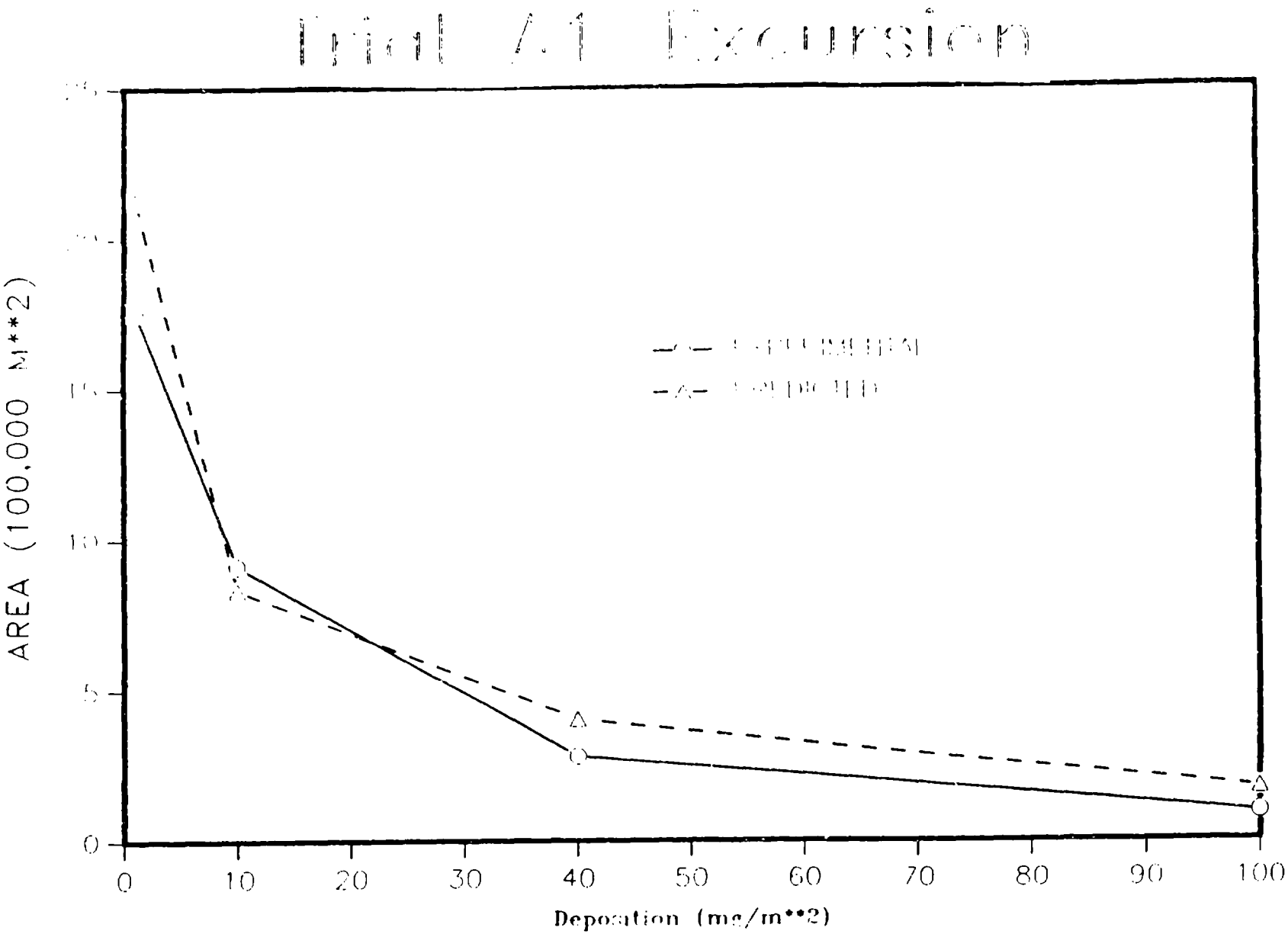
AREA (100,000 M**2)
0
5
10
Deposition (mg/m**2)
0
10
20
30
40
50
60
70
80
90
100

Figure B-4

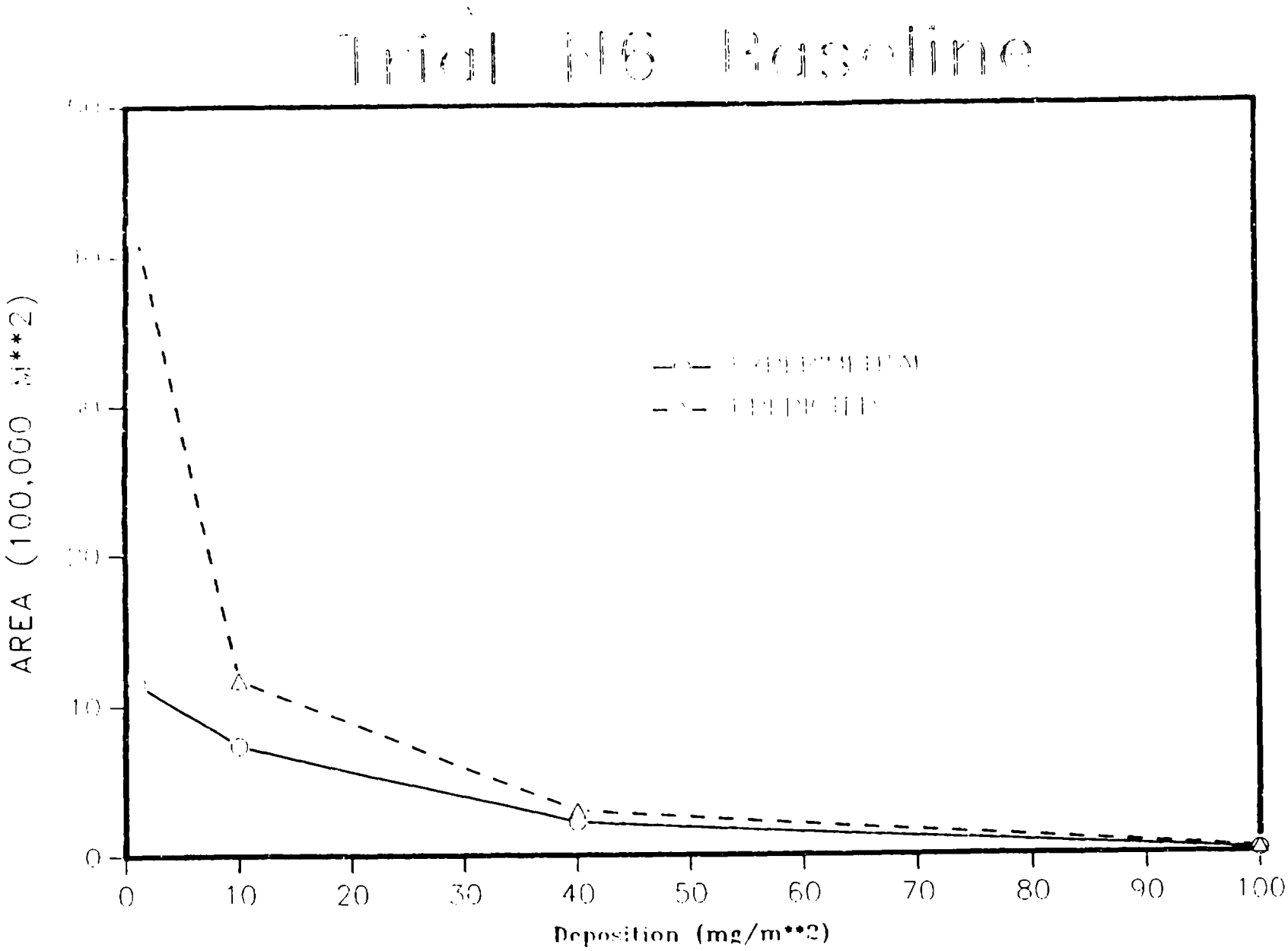
Trial #6 Baseline
AREA (100,000 M**2)
0
10
20
30
40
50
60
70
80
90
100
Deposition (mg/m**2)

Figure B-5

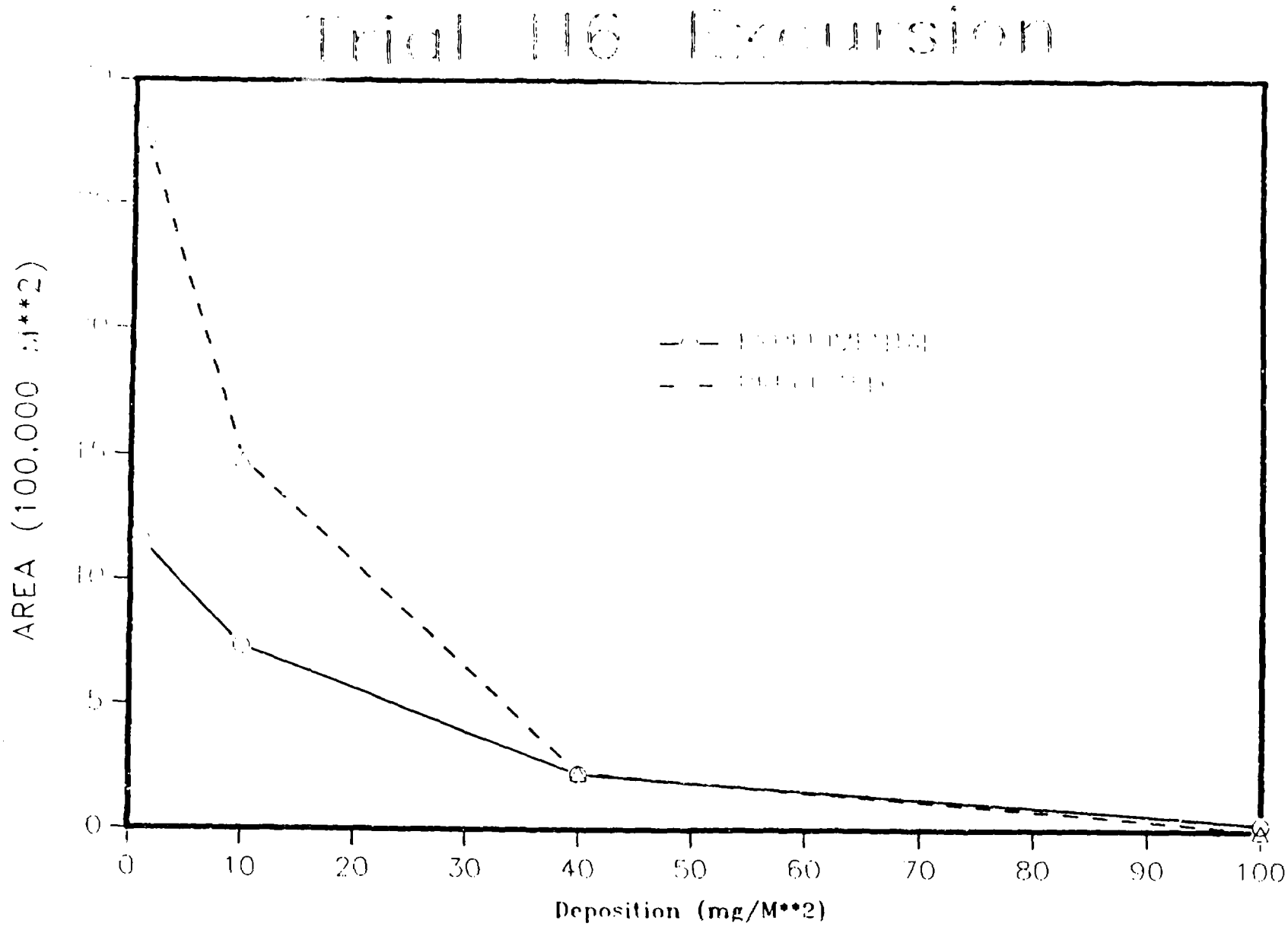
Trial 116 Excursion
AREA (100,000 M**2)
0
5
10
15
0
10
20
30
40
50
60
70
80
90
100
Deposition (mg/M**2)

Figure B-6

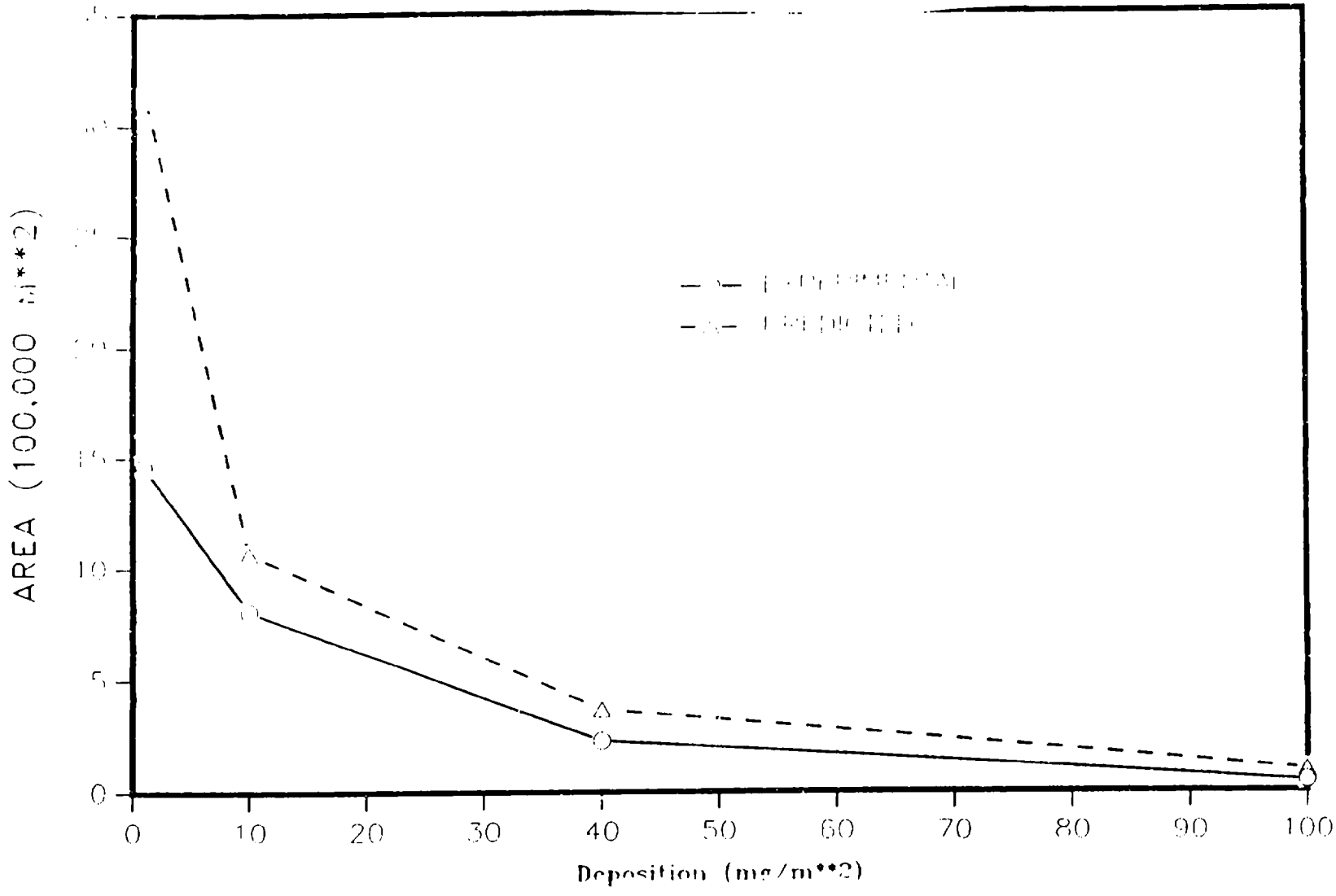

Figure B-7

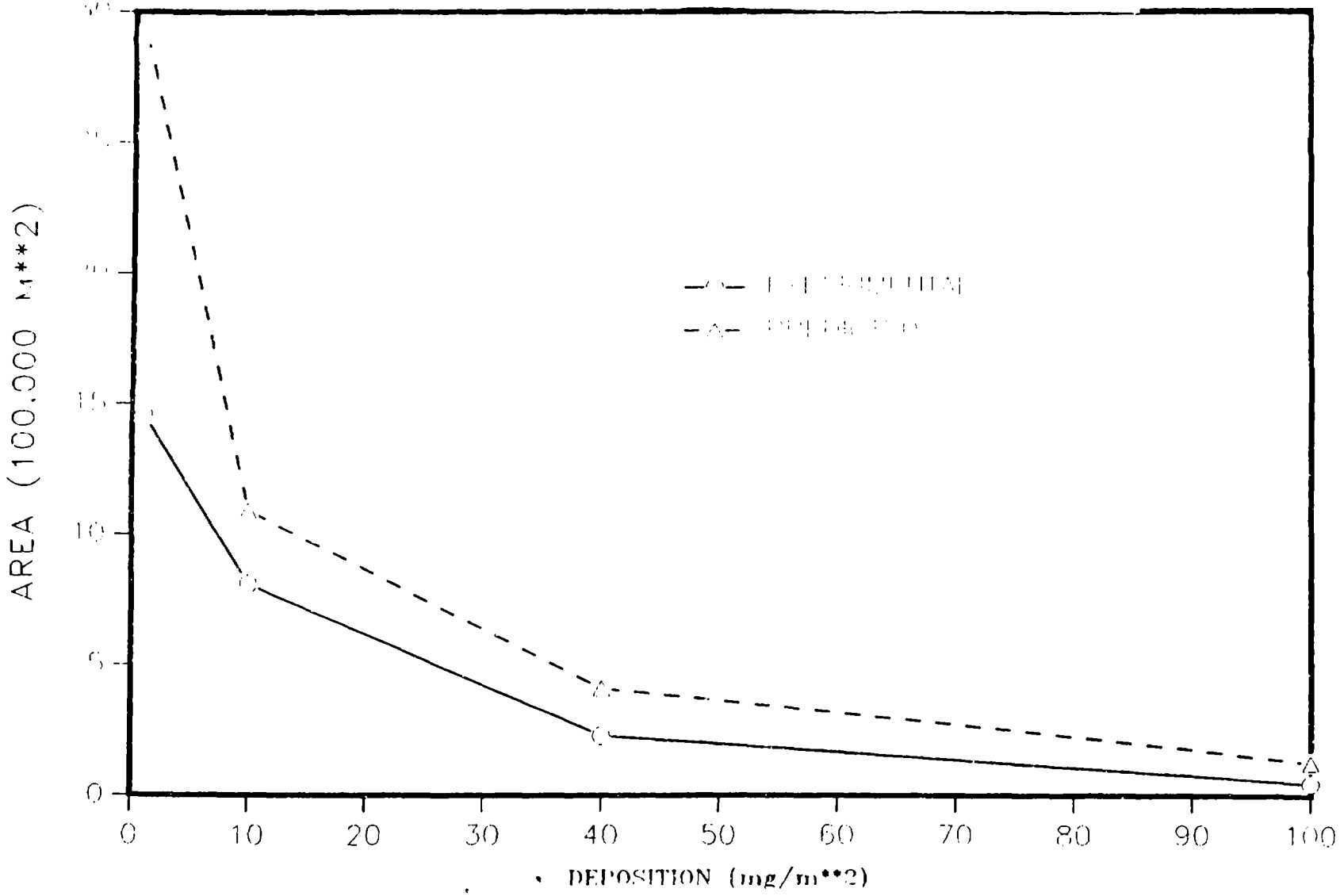
AREA (100,000 M**2)
0
5
10
15
0
10
20
30
40
50
60
70
80
90
100
DEPOSITION (mg/m**2)

Figure B-8

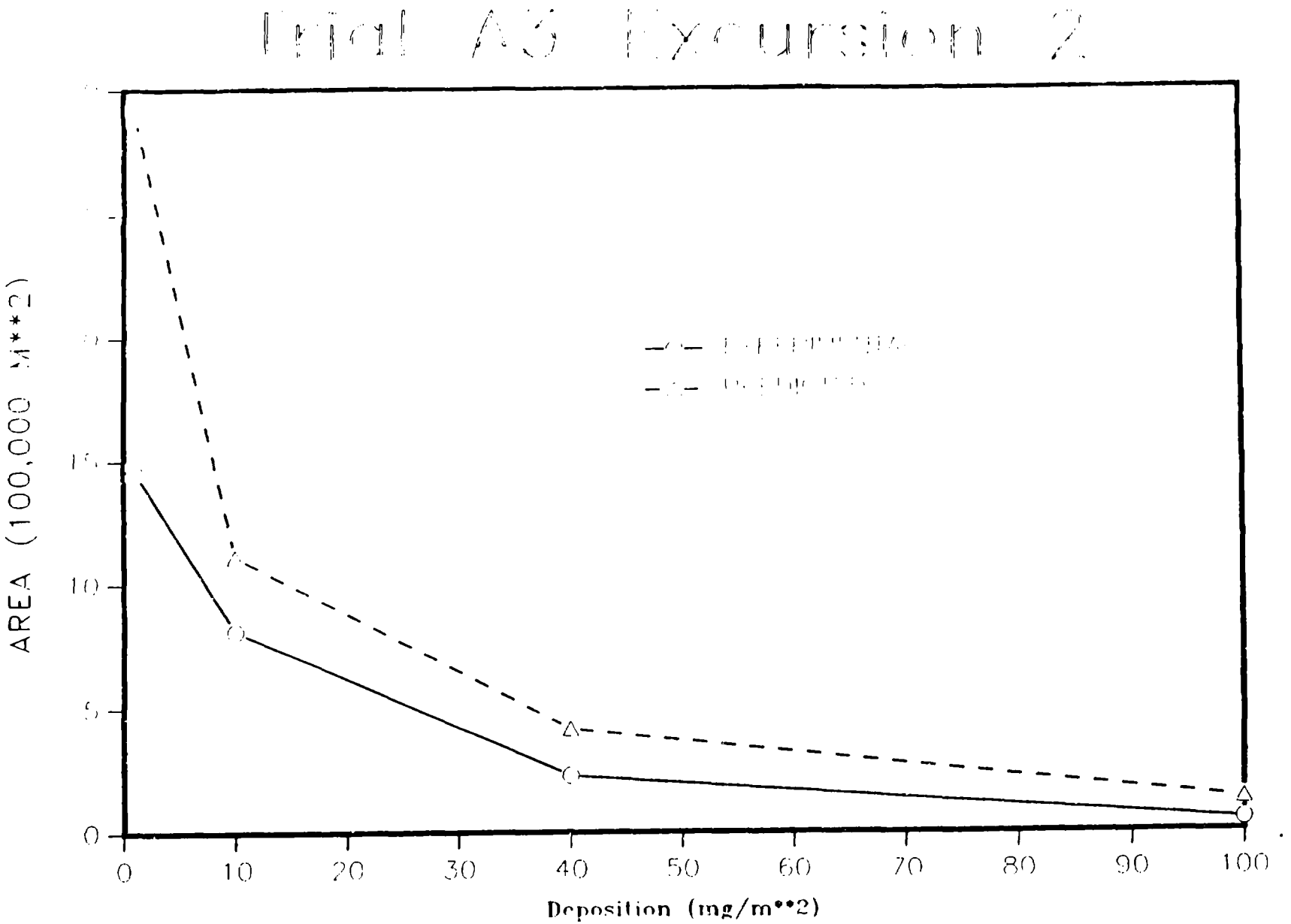
AREA (100,000 M**2)
0
5
10
Deposition (mg/m**2)
0
10
20
30
40
50
60
70
80
90
100

Figure B-9

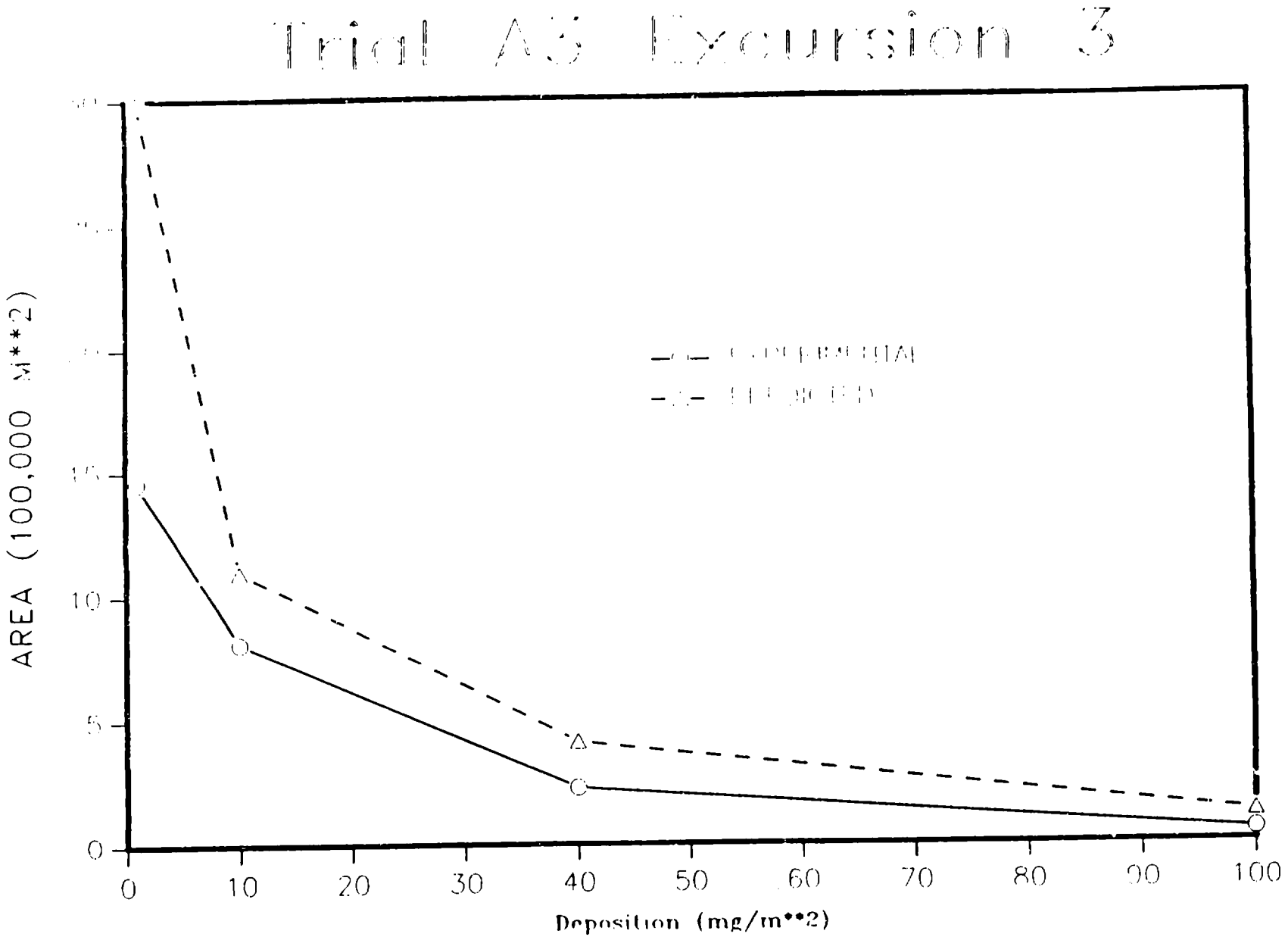
Trial A3 Excursion 3
AREA (100,000 M**2)
0
5
10
0
10
20
30
40
50
60
70
80
90
100
Deposition (mg/m**2)

Figure B-10

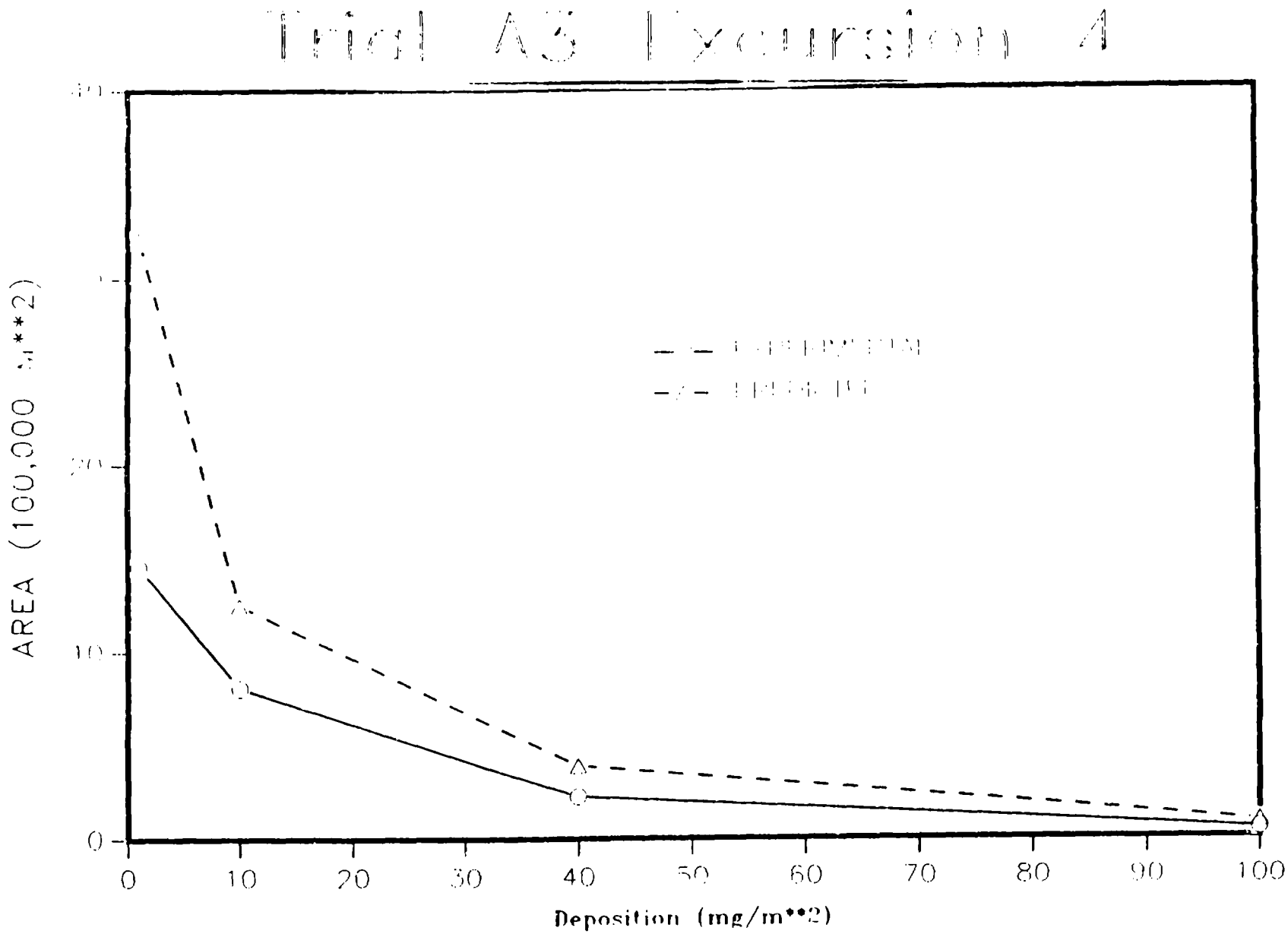
Trial A3 Excursion 4
AREA (100,000 m**2)
0
10
20
0
10
20
30
40
50
60
70
80
90
100
Deposition (mg/m**2)

Figure B-11

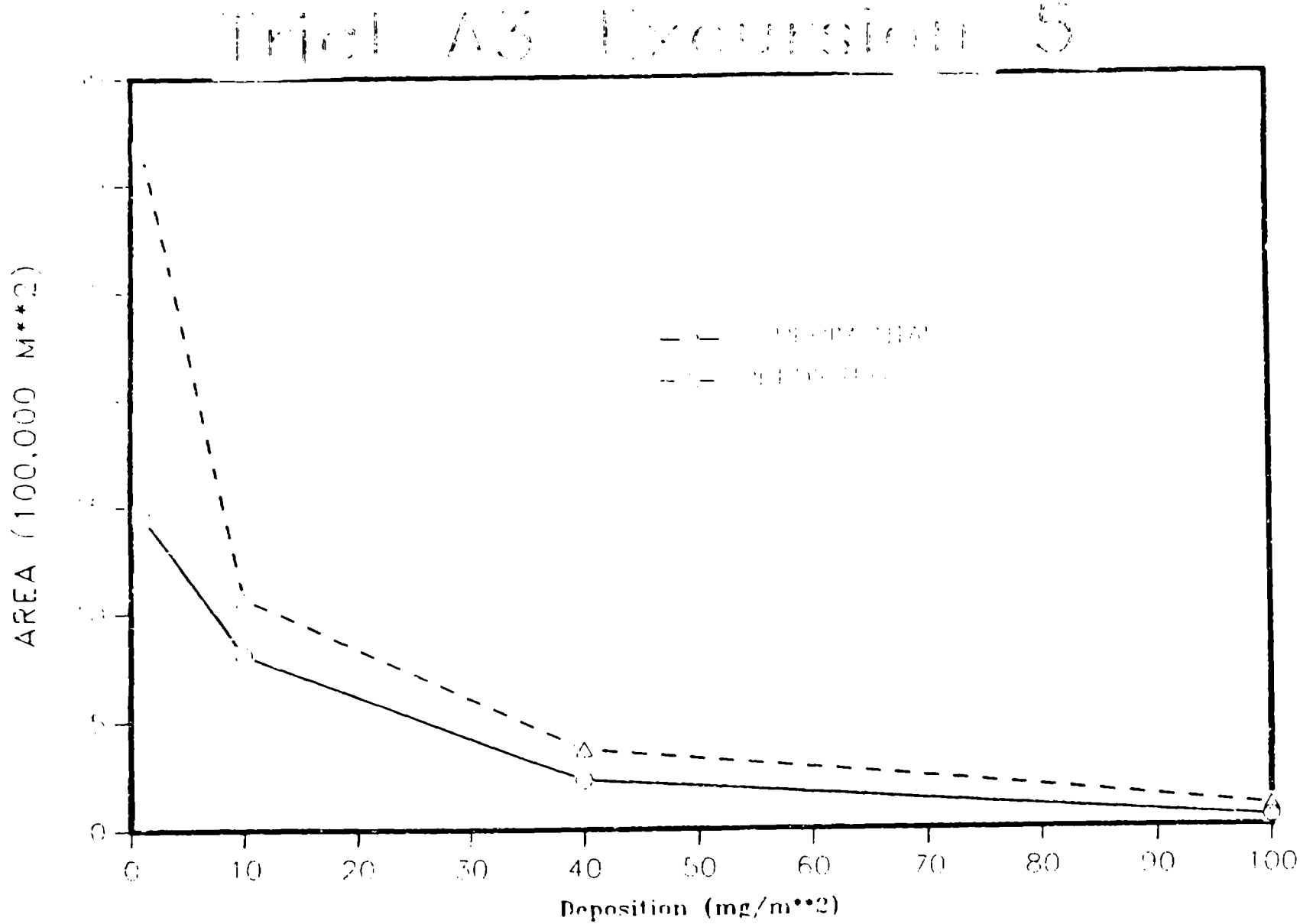

Figure B-12

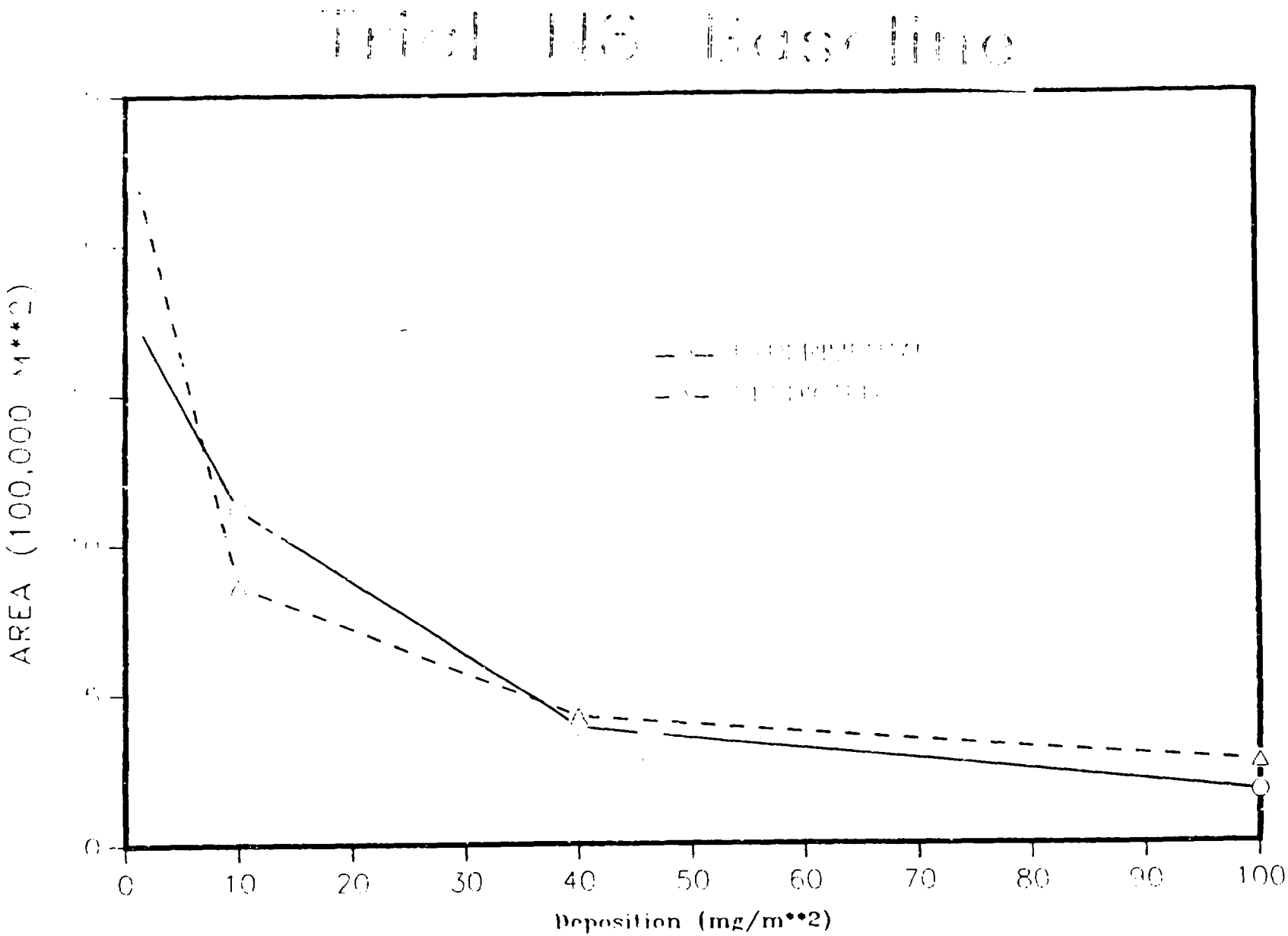

Figure B-13

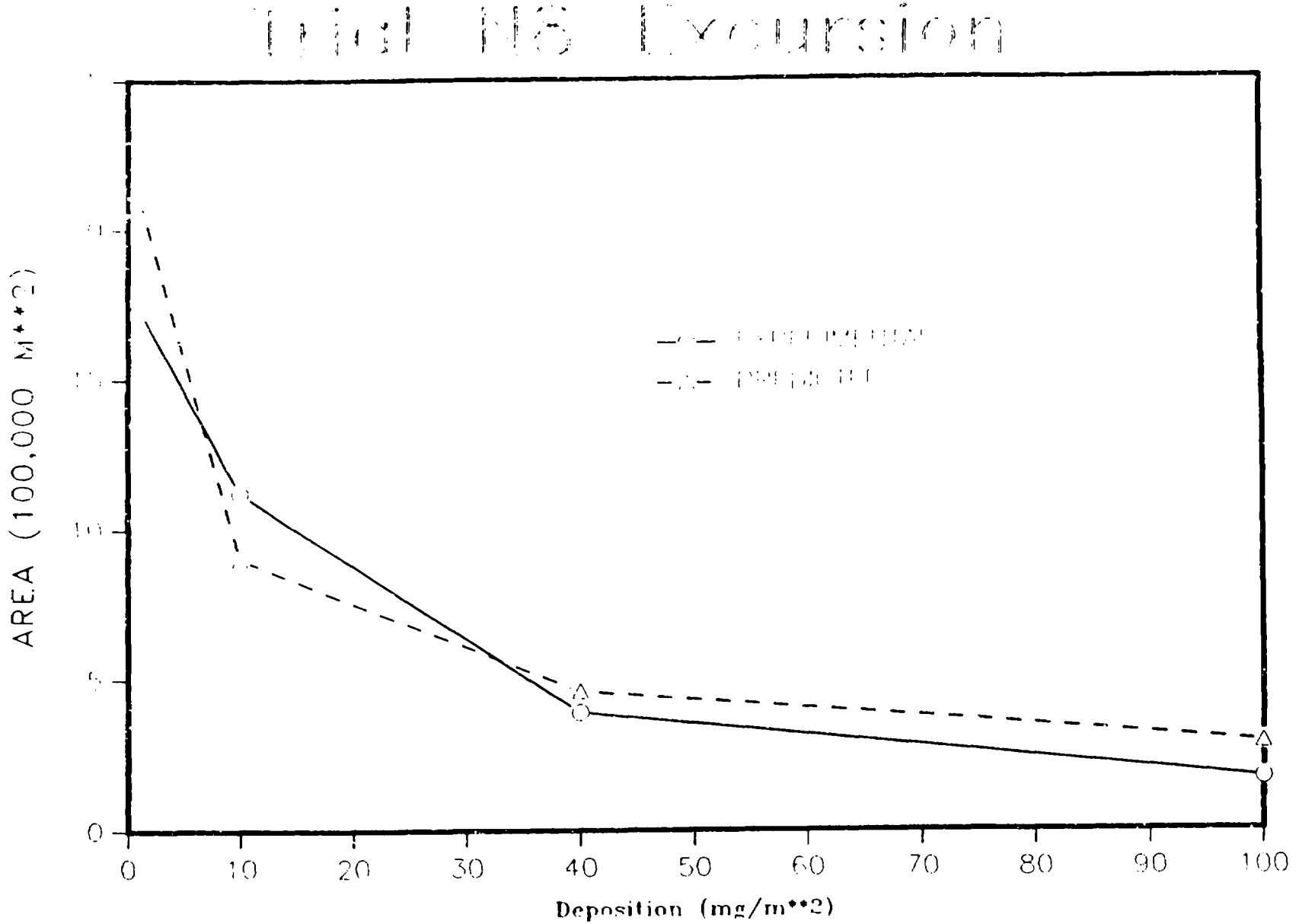

Figure B-14

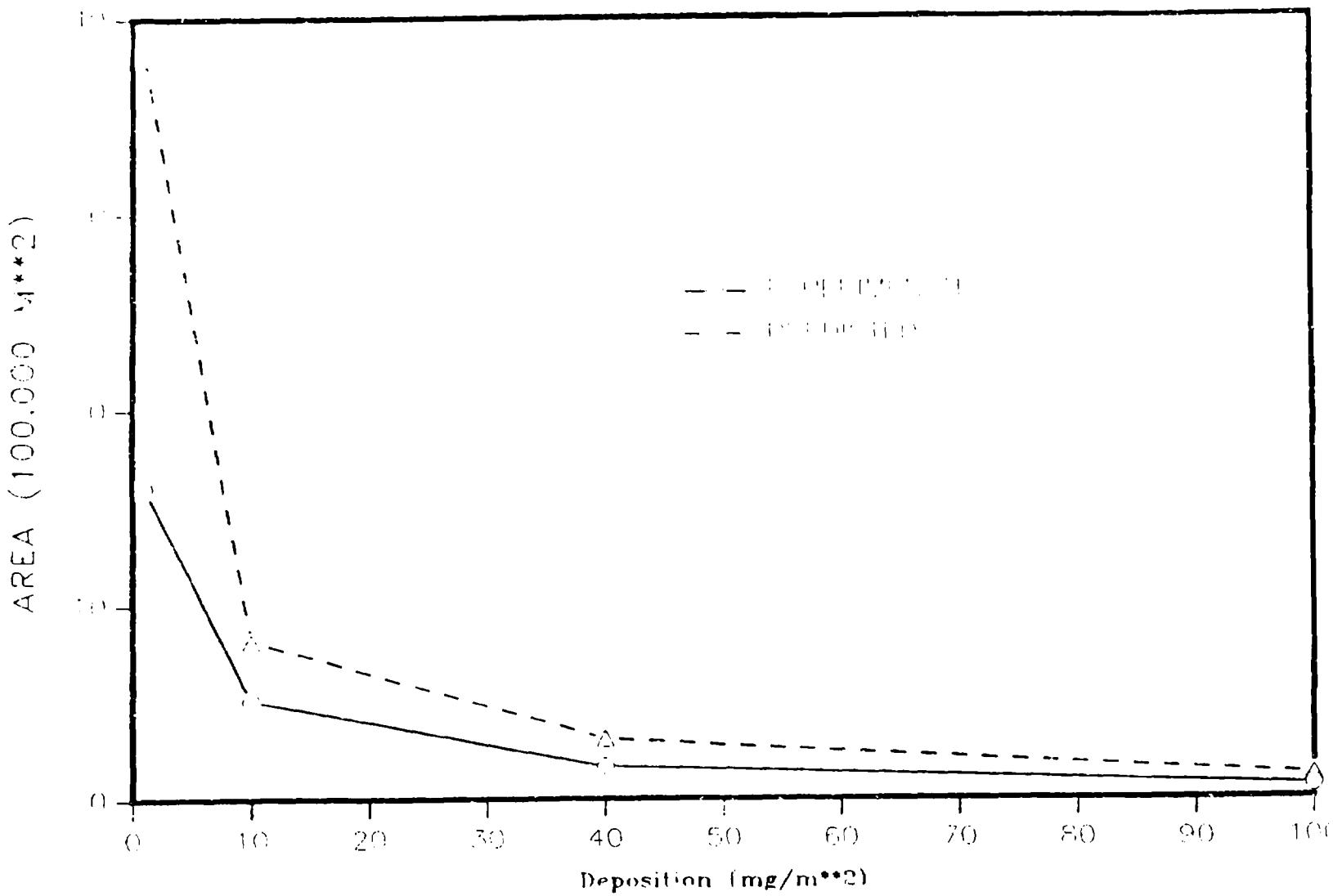

Figure B-15

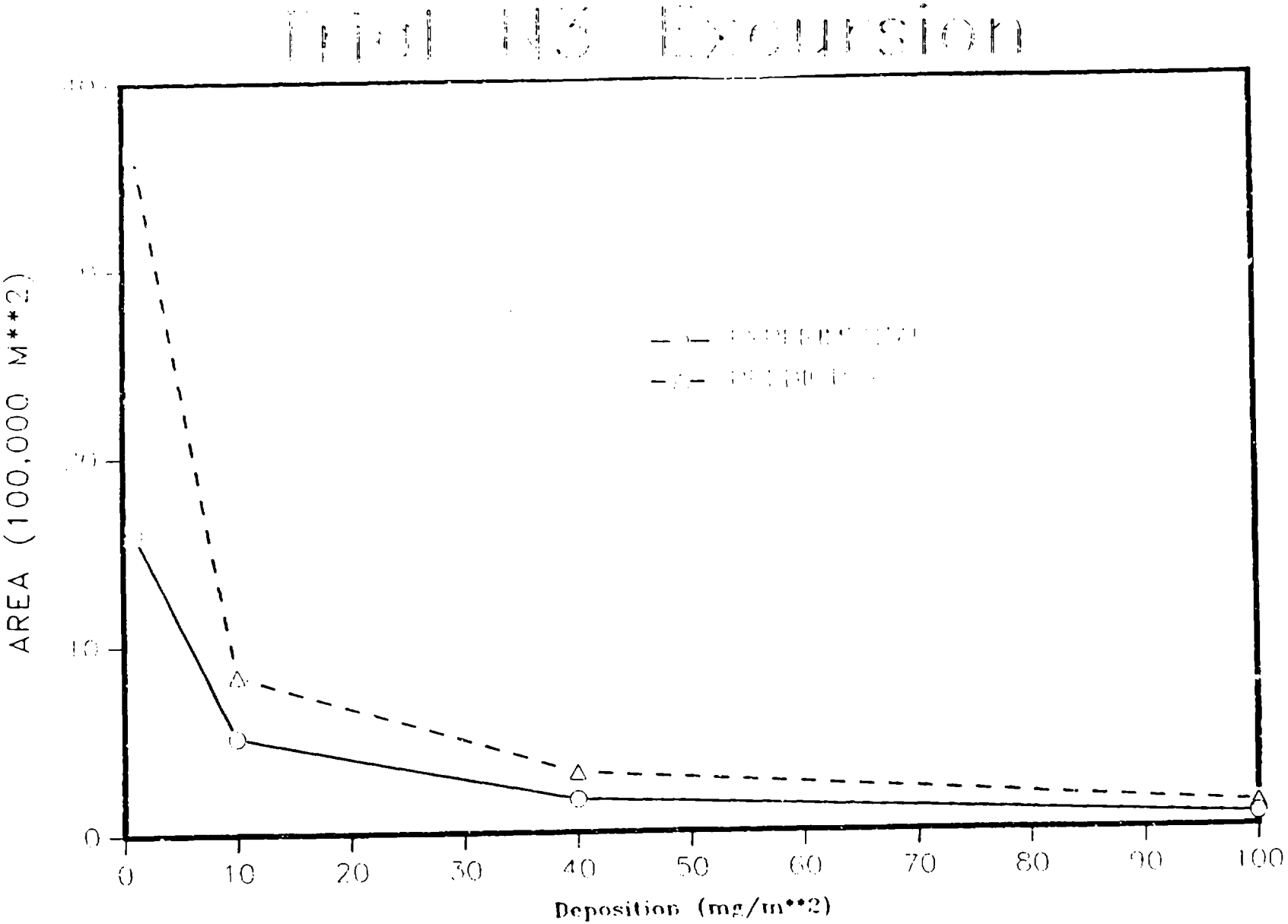
AREA (100,000 M**2)
0
10
0
10
20
30
40
50
60
70
80
90
100
Deposition (mg/m**2)

Figure B-16

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